UNIVERSITY OF ARKANSAS

AM³ Lab
Advanced Manufacturing | Modeling | Materials

Additive Manufacturing – Module 8

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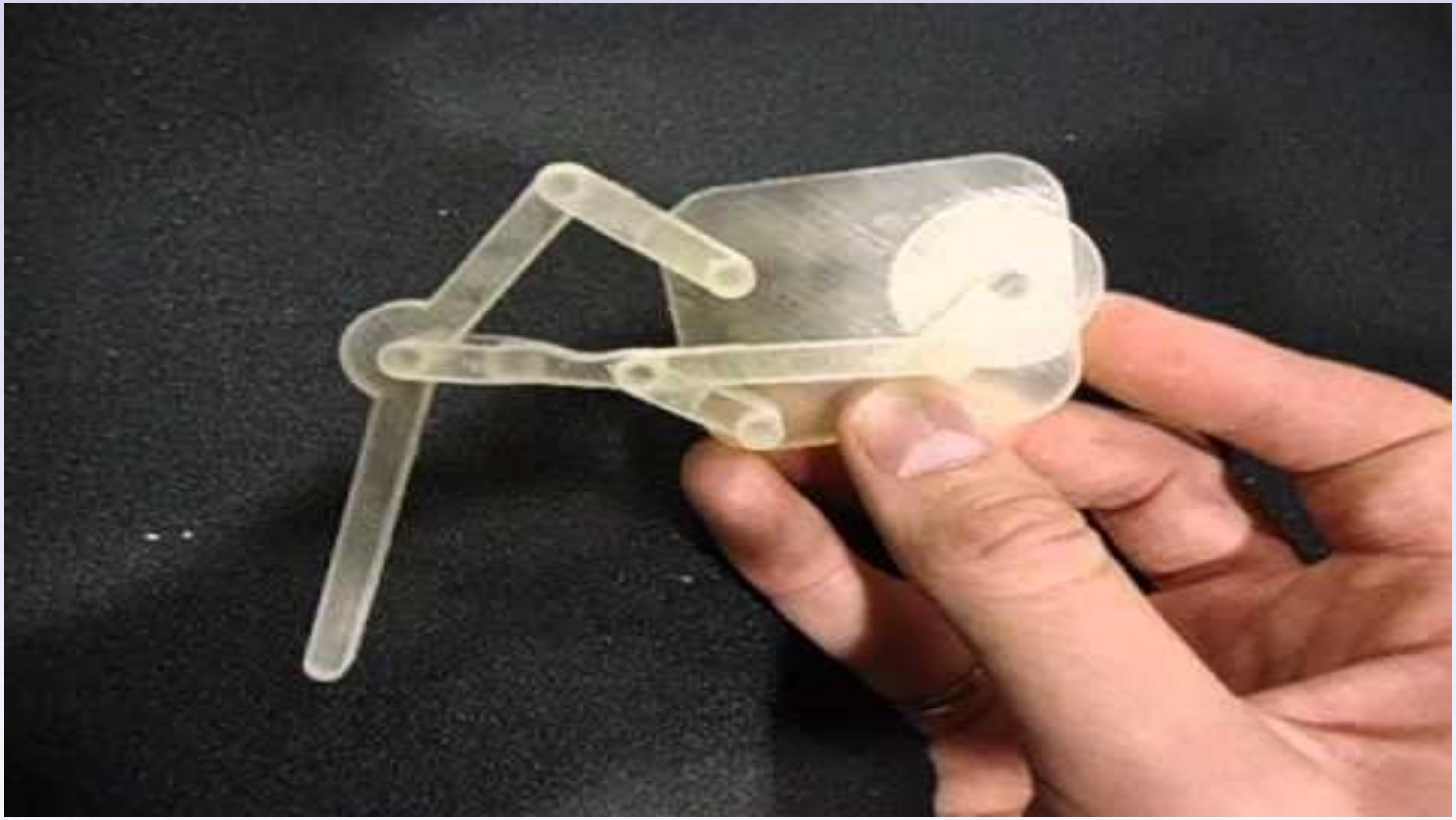
CAE

Evaluating design



https://www.youtube.com/watch?v=p__-QbQbntI

A design of a motion system – motion can be described using kinematic equations when approximated as rigid structures

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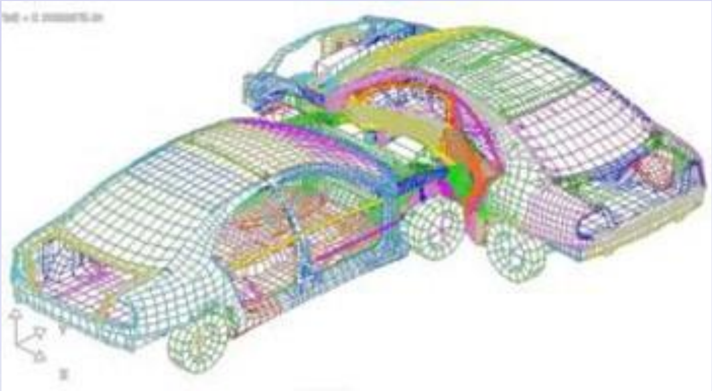
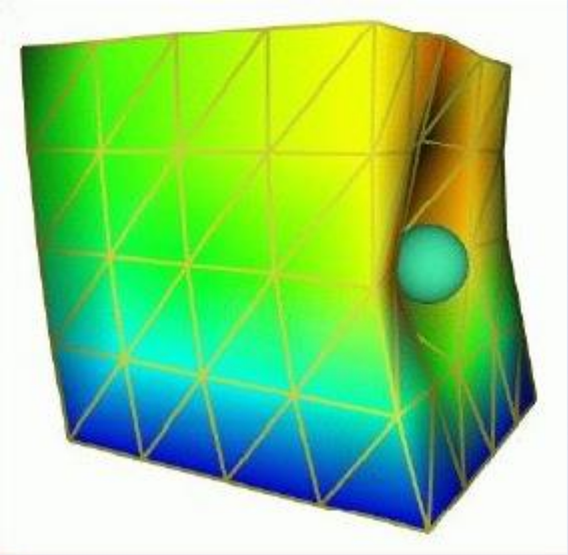
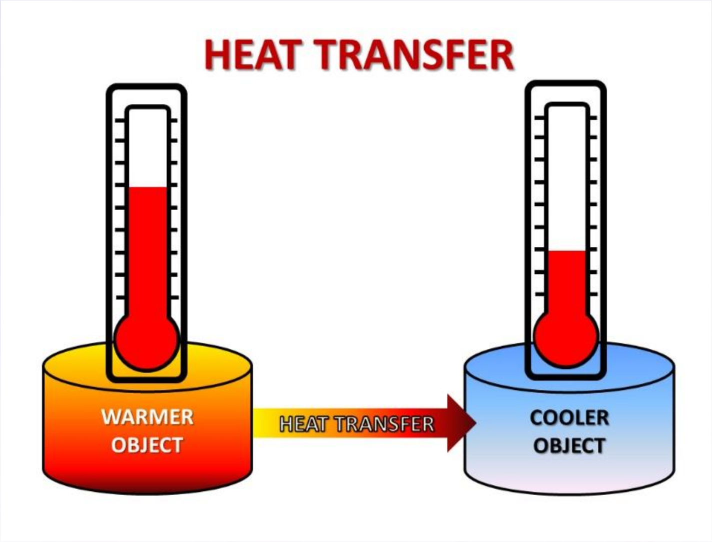
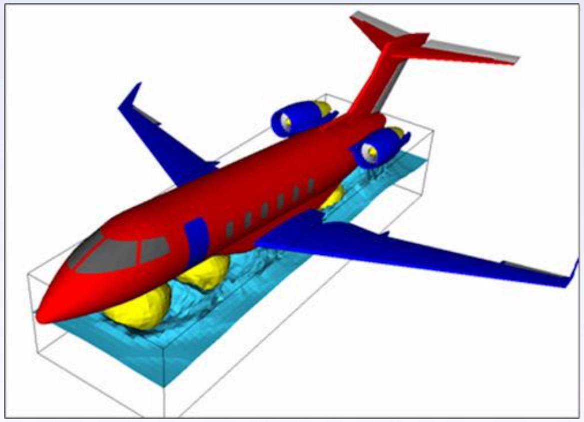
Evaluating design









What if your design is deformable structure, involves heat transfer, or fluids

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FDM
FEM

Evaluating design

- Conservation Equations
  - Conservation of Mass
  - Conservation of Energy
  - Conservation of Momentum

⇩

- Partial Differential Equations
  - Describing change in space and time

- Constitutive Models for Materials
  - Hooke's Law
  - Newtonian Fluid
  - Etc.

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Evaluating design

Millennium Prize Problems

P versus NP problem
Hodge conjecture
Poincaré conjecture (solved)
Riemann hypothesis
Yang–Mills existence and mass gap
Navier–Stokes existence and smoothness
Birch and Swinnerton-Dyer conjecture

V · T · E

Even much more basic properties of the solutions to Navier–Stokes have never been proven. For the three-dimensional system of equations, and given some initial conditions, **mathematicians have not yet proved that smooth solutions always exist**, or that if they do exist, they have bounded energy per unit mass.

What about higher order, higher dimension PDEs

$$F\left(x_1, \ldots, x_n, u, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_n}, \frac{\partial^2 u}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 u}{\partial x_1 \partial x_n}, \ldots\right) = 0.$$

Reality: Most PDEs CANNOT be solved analytically!!!

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Evaluating design

- Numerical solutions
  - Discretize and turn PDEs into a system of algebraic equations (mostly linear)

Most popular methods

- Finite difference methods
- Finite element methods

Other methods

- Finite volume method
- Boundary element method
- Discrete element method
- Spectral method
- Particle based methods

http://en.wikipedia.org/wiki/List_of_numerical_analysis_topics#Numerical_methods_for_partial_differential_equations

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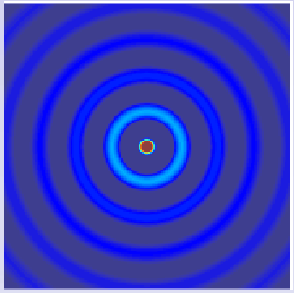
Classification of PDEs

Second-order linear PDEs

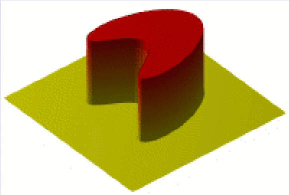
$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu + g = 0$$

are classified based on the value of the discriminant $b^2 - 4ac$

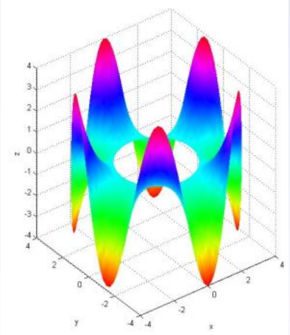
- $b^2 - 4ac > 0$: hyperbolic
  - e.g., wave equation: $u_{tt} - u_{xx} = 0$
  - Hyperbolic PDEs describe time dependent, conservative physical processes, such as convection, that are not evolving toward steady state.
- $b^2 - 4ac = 0$: parabolic
  - e.g., heat equation: $u_t - u_{xx} = 0$
  - Parabolic PDEs describe time-dependent dissipative physical processes, such as diffusion, that are evolving toward steady state.
- $b^2 - 4ac < 0$: elliptic
  - e.g., Laplace equation: $u_{xx} + u_{yy} = 0$
  - Elliptic PDEs describe processes that have already reached steady states, and hence are time-independent.



Wave equation



Heat equation



Laplace equation

Finite Difference Method

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x)}{dx}$$

Discretize

$$\partial_x f^{+} \approx \frac{f(x+dx) - f(x)}{dx}$$

Forward difference

$$\partial_x f^{-} \approx \frac{f(x) - f(x-dx)}{dx}$$

Backward difference

$$\partial_x f \approx \frac{f(x+dx) - f(x-dx)}{2dx}$$

Centered difference

Finite Difference Method

- **Consider a 1D initial-boundary value problem for heat equation**

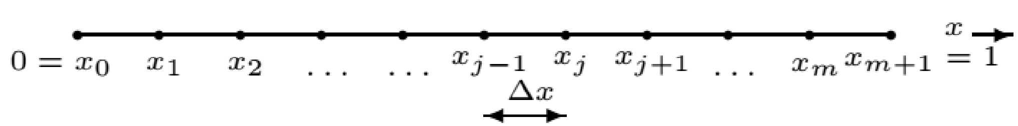
$$u_t = \kappa u_{xx},\ 0 \le x \le 1,\ t \ge 0$$

$$u(0, x) = f(x),\ \text{Initial Condition}$$

$$u(t, 0) = \alpha,\ \text{Boundary Condition at } x = 0$$

$$u(t, 1) = \beta,\ \text{Boundary Condition at } x = 1$$

Discretize the spatial domain $[0, 1]$ into $m + 2$ grid points using a uniform mesh step size $\boxed{\Delta x = 1/(m+1)}$. Denote the spatial grid points by $x_j, j = 0, 1, \ldots m + 1$.



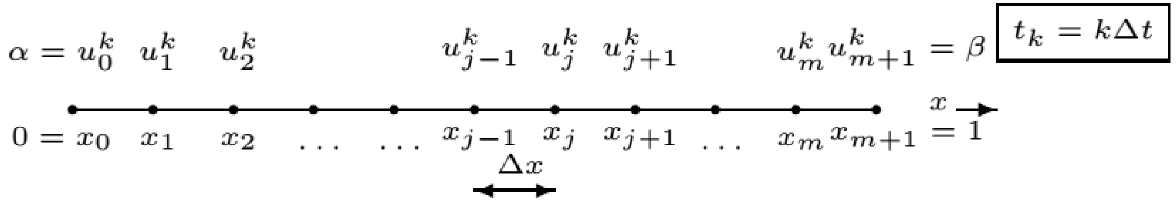
Credit: Vrushali A. Bokil and Nathan L. Gibson @ Oregon State U

Finite Difference Method

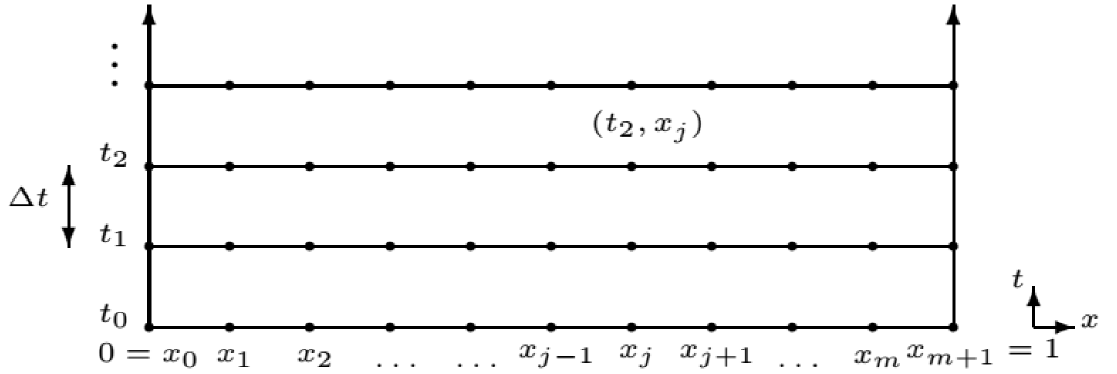
Consider a 1D initial-boundary value problem for heat equation

Similarly discretize the temporal domain into temporal grid points $t_k = k\Delta t$ for suitably chosen time step Δt.

Denote the approximate solution at the grid point (t_k, x_j) as U_j^k.



The space-time grid can be represented as



Credit: Vrushali A. Bokil and Nathan L. Gibson @ Oregon State U

Finite Difference Method

Consider a 1D initial-boundary value problem for heat equation

Replace u_t by a forward difference in time and u_{xx} by a central difference in space to obtain the explicit FDM

$$\frac{U_j^{k+1}-U_j^k}{\Delta t}=\kappa\frac{U_{j+1}^k-2U_j^k+U_{j-1}^k}{(\Delta x)^2}$$

$$\Longrightarrow U_j^{k+1}=U_j^k+\frac{\kappa\Delta t}{(\Delta x)^2}\left(U_{j+1}^k-2U_j^k+U_{j-1}^k\right),\ j=1,2,\ldots m$$

Using Taylor series to determine order of accuracy for the approximation

$$f(x\pm dx)=f(x)\pm \mathrm{dx}f'(x)+\frac{dx^2}{2!}f''(x)\pm\frac{dx^3}{3!}f'''(x)+\frac{dx^4}{4!}f''''(x)\pm\ldots$$

First order accurate in time

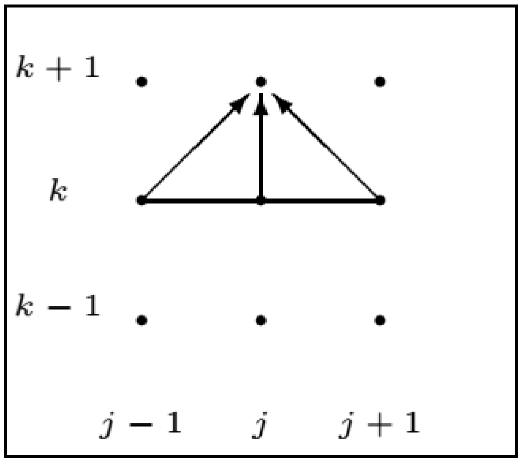
$$\frac{f(x+dx)-f(x)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f'(x)+\frac{dx^2}{2!}f''(x)+\frac{dx^3}{3!}f'''(x)+\ldots\right]$$
$$=f'(x)+O(dx)$$

Second order accurate in space

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_i=\frac{u_{i+1}-2u_i+u_{i-1}}{(\Delta x)^2}+O((\Delta x)^2)$$

Finite Difference Method

- **Consider a 1D initial-boundary value problem for heat equation**



Computational Stencil

The local truncation error is $O(\Delta t) + O((\Delta x)^2)$.

- **How to choose Δt and Δx?**

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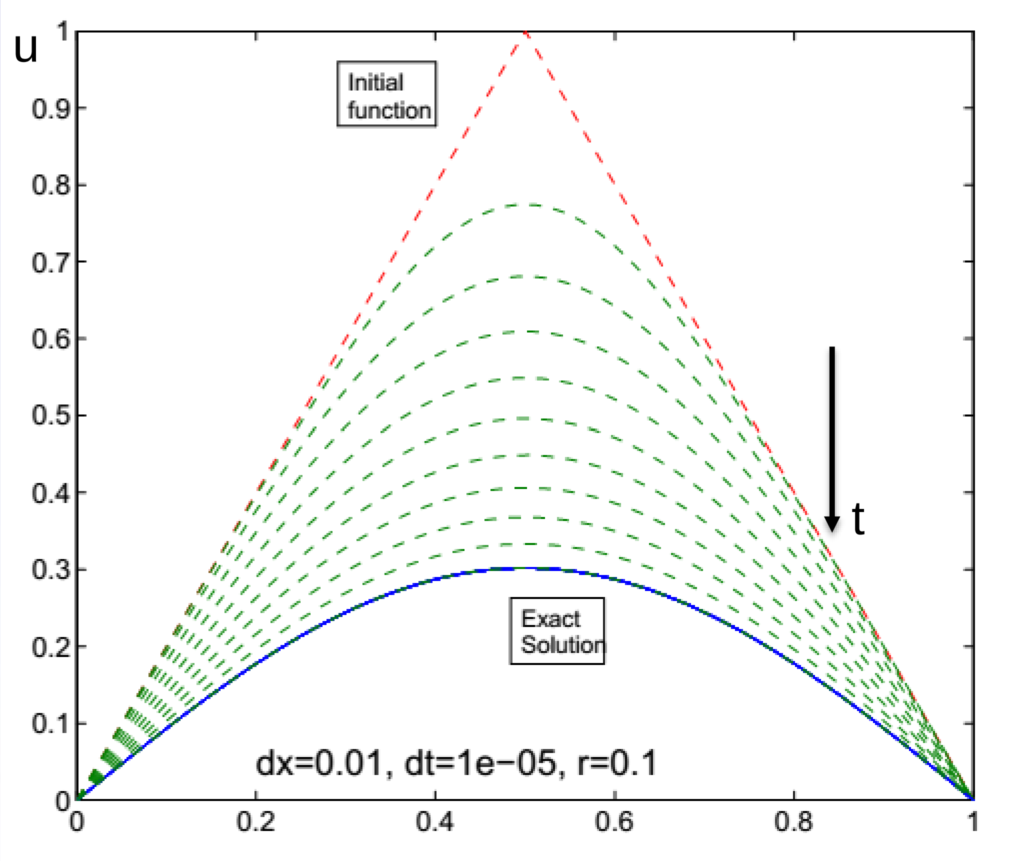
Finite Difference Method

- **How to choose Δt and Δx?**



$$r = \frac{\kappa \Delta t}{\Delta x} \leq \frac{1}{2}$$

With $\Delta x = 0.01$ and $\Delta t = 10^{-5}$

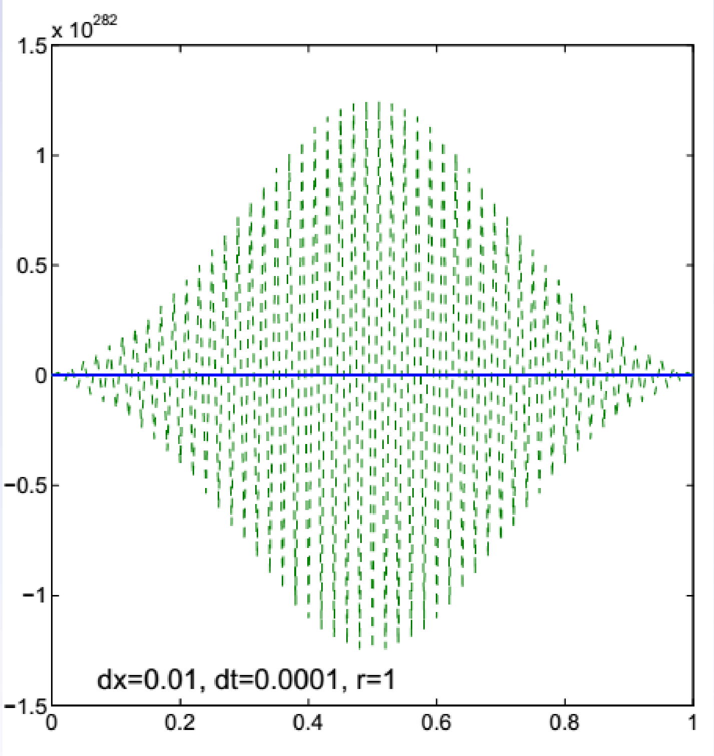
What happens if r is greater than 1/2?

- **Initial condition: discontinuous at x = 0.5**
- **Rapid smoothing of discontinuity as time evolves**
- **High frequency damps quickly. The heat equation is stiff**

Finite Difference Method

- **How to choose Δt and Δx?**

What happens if r is greater than 1/2?



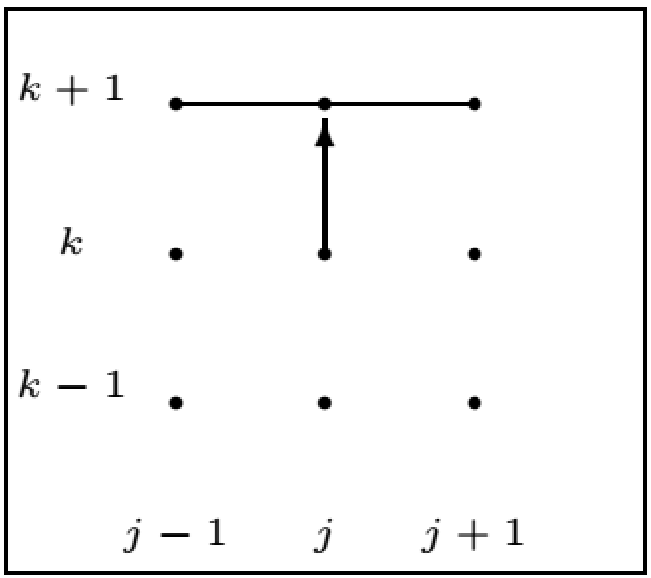
- **Unstable behavior of numerical solution**
- **Δt and Δx cannot be chosen arbitrarily. Must satisfy a stable condition.**

Finite Difference Method

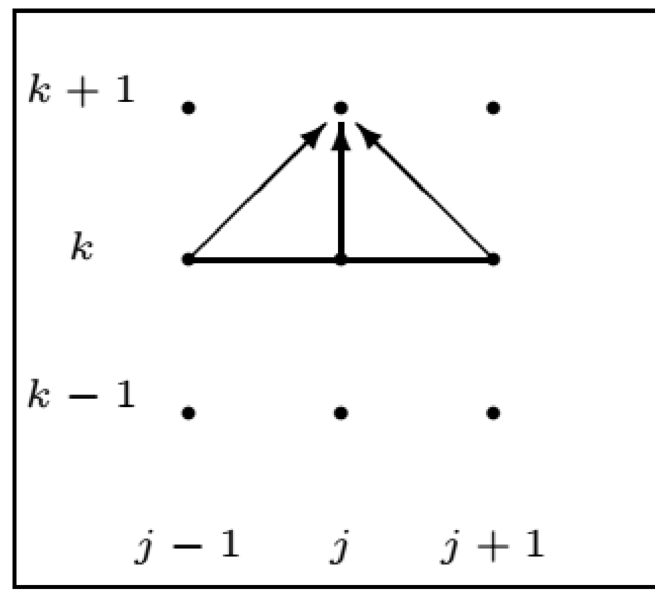
Implicit FDM

$$\frac{U_j^{k+1} - U_j^k}{\Delta t} = \kappa \frac{U_{j+1}^{k+1} - 2U_j^{k+1} + U_{j-1}^{k+1}}{(\Delta x)^2}$$

$$\Longrightarrow \quad U_j^{k+1} = U_j^k + \frac{\kappa \Delta t}{(\Delta x)^2}\left(U_{j+1}^{k+1} - 2U_j^{k+1} + U_{j-1}^{k+1}\right), \; j = 1, 2, \ldots m$$



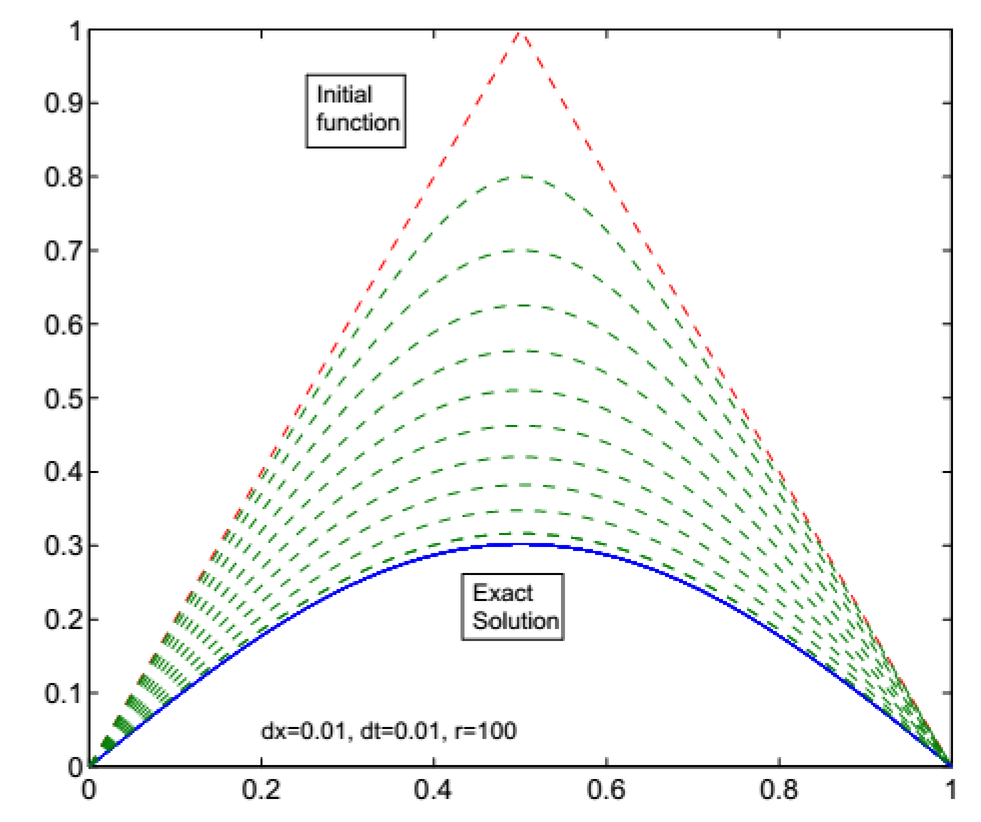
Implicit computational stencil



Explicit computational stencil

Finite Difference Method

Implicit FDM



- **Stable behavior of numerical solution**
- **Δt and Δx cannot be chosen to have the same order of magnitude. Unconditionally stable.**

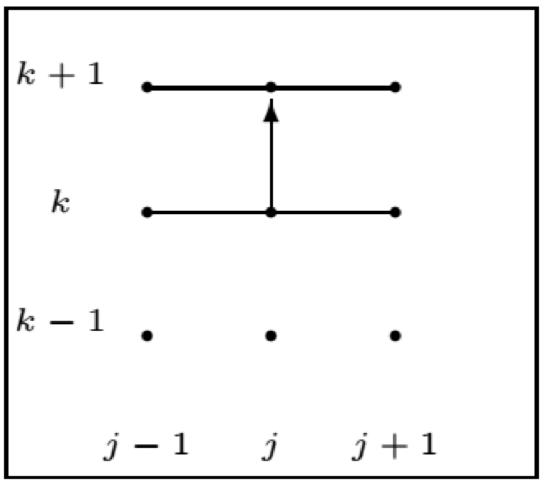
Finite Difference Method

- **Implicit FDM – 2nd order accurate in time – trapezoid rule**

$$\frac{U_j^{k+1}-U_j^k}{\Delta t}=\frac{\kappa}{2}\left(\frac{U_{j+1}^k-2U_j^k+U_{j-1}^k}{(\Delta x)^2}\right)+\frac{\kappa}{2}\left(\frac{U_{j+1}^{k+1}-2U_j^{k+1}+U_{j-1}^{k+1}}{(\Delta x)^2}\right)$$

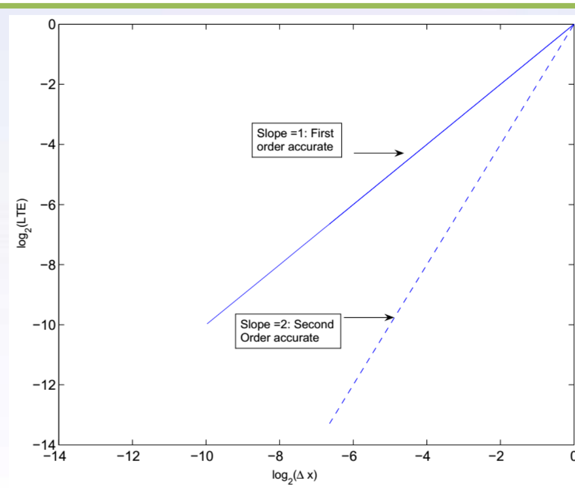
$$\Longrightarrow U_j^{k+1}=U_j^k+\frac{\kappa\Delta t}{2(\Delta x)^2}\left(U_{j+1}^k-2U_j^k+U_{j-1}^k+U_{j+1}^{k+1}-2U_j^{k+1}+U_{j-1}^{k+1}\right),$$

$$j=1,2,\ldots m$$



Computational stencil

- **Unconditionally stable**
- **Second order accurate in time**

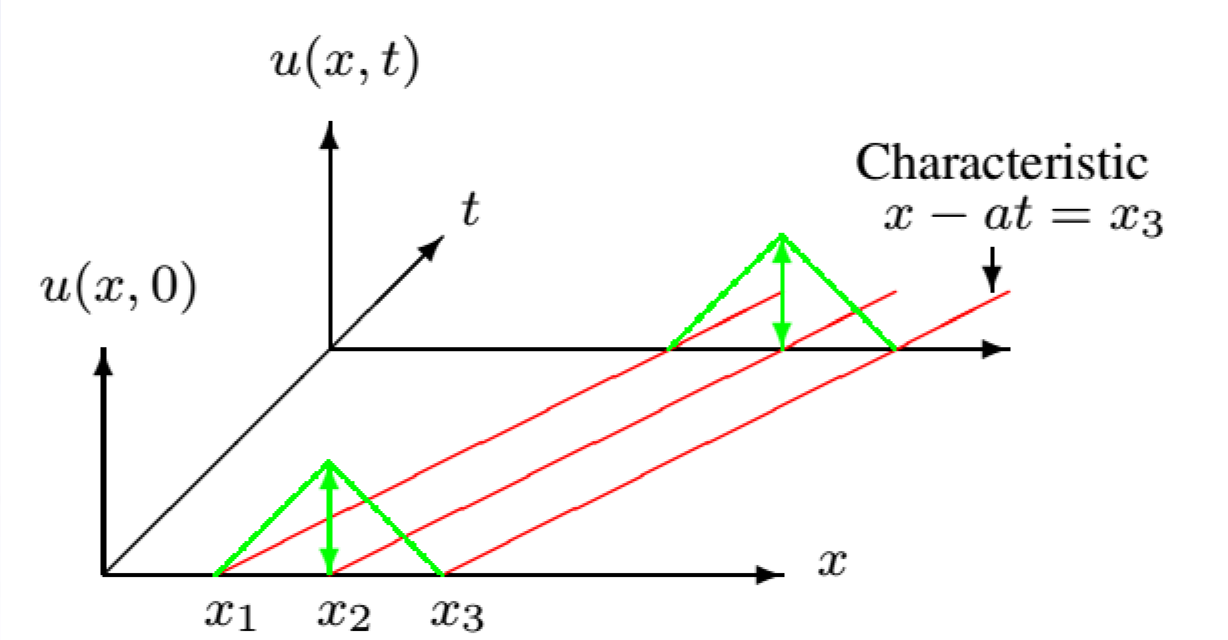


Finite Difference Method

FDM for advection equation

$$u_t + a u_x = 0,\ 0 \le x \le 1,\ t \ge 0$$

$$u(0,x) = f(x),\ \text{Initial Condition}$$



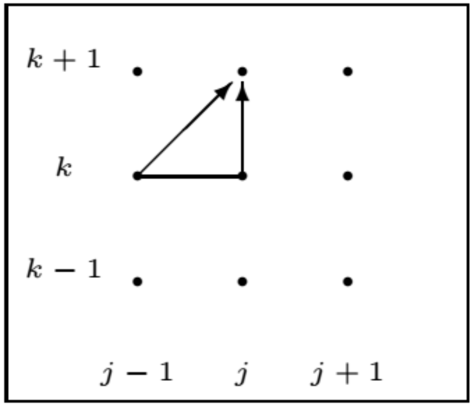
Information propagates along characteristics

Finite Difference Method

FDM for advection equation

$$\frac{U_j^{k+1} - U_j^k}{\Delta t} + a\frac{U_{j+1}^k - U_j^k}{\Delta x} = 0$$

$$\Longrightarrow \quad U_j^{k+1} = U_j^k + \frac{a\Delta t}{\Delta x}\left(U_j^k - U_{j-1}^k\right), \; j = 1, 2, \ldots m$$



Computational stencil

- **Scheme is explicit**
- **First order accurate in space and time**
- **Δt and Δx are related by CFL number: $\nu = a\Delta t / \Delta x$**

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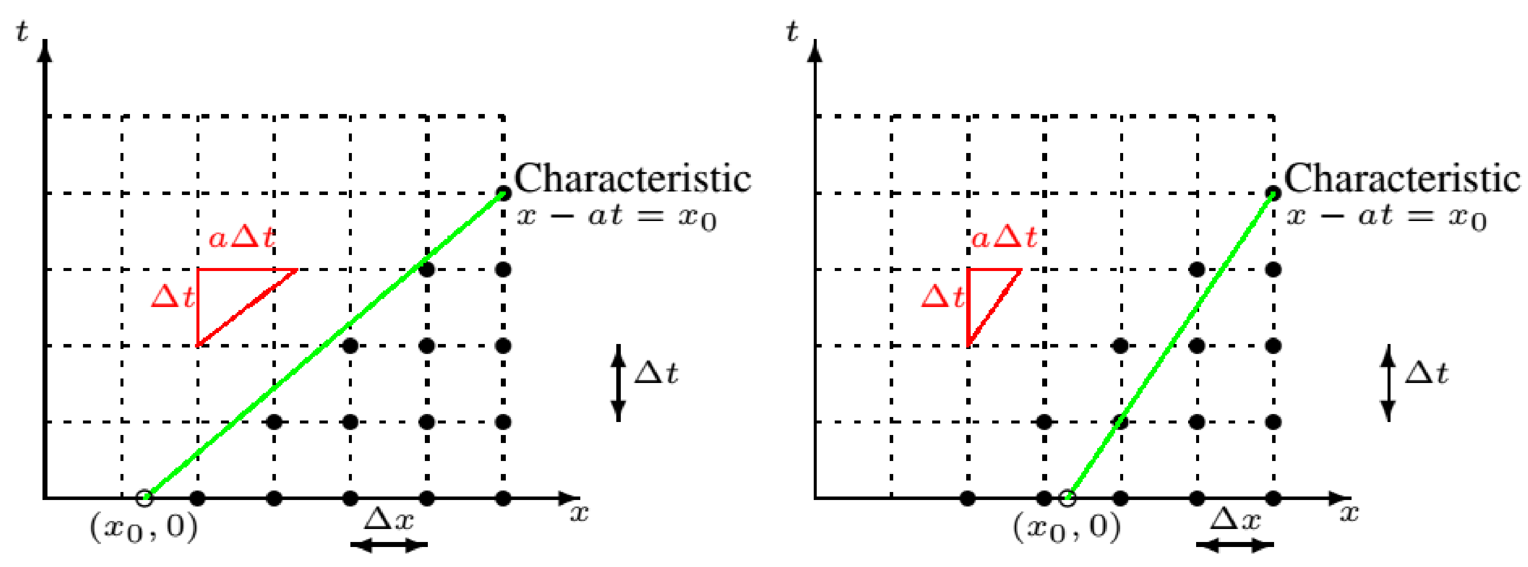
Finite Difference Method

FDM for advection equation

The CFL Condition: For stability, at each mesh point, the Domain of dependence of the PDE must lie within the domain of dependence of the numerical scheme.

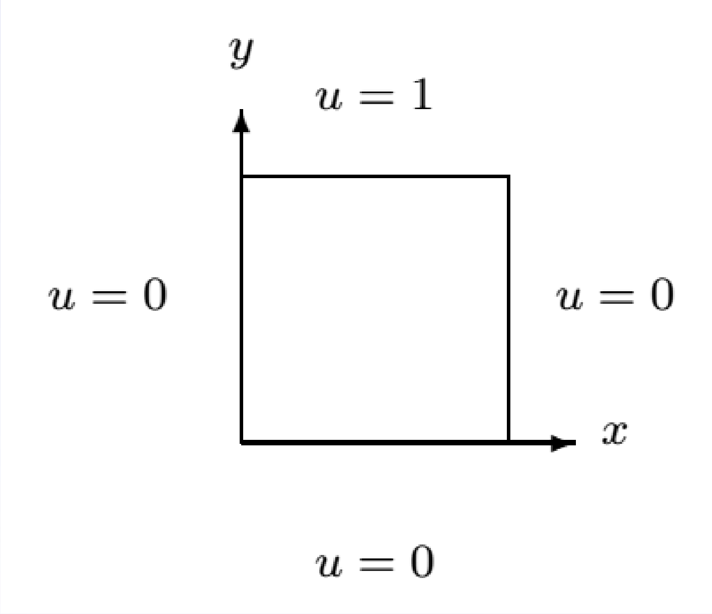


- CFL $\nu <= 1$
- CFL is a necessary condition for stability of explicit FDM applied to Hyperbolic PDEs. It is not a sufficient condition.

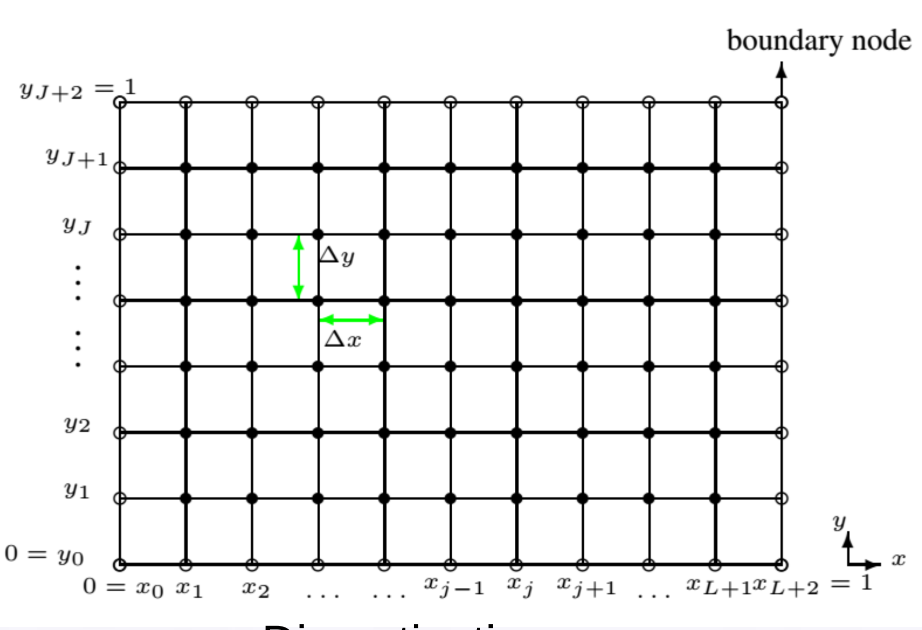
Finite Difference Method

FDM for Laplace equation

$$u_{xx} + u_{yy} = 0,\ 0 \le x \le 1,\ 0 \le y \le 1$$



Boundary conditions



Discretization

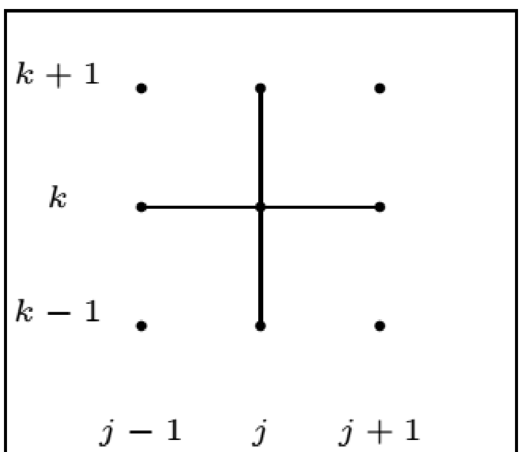
Finite Difference Method

FDM for Laplace equation – centered difference scheme

$$\frac{U_{j+1,k} - 2U_{j,k} + U_{j-1,k}}{(\Delta x)^2} + \frac{U_{j,k+1} - 2U_{j,k} + U_{j,k-1}}{(\Delta y)^2} = 0$$

If $\Delta x = \Delta y$ this becomes

$$U_{j+1,k} + U_{j-1,k} + U_{j,k+1} + U_{j,k-1} - 4U_{j,k} = 0$$



Five-point stencil

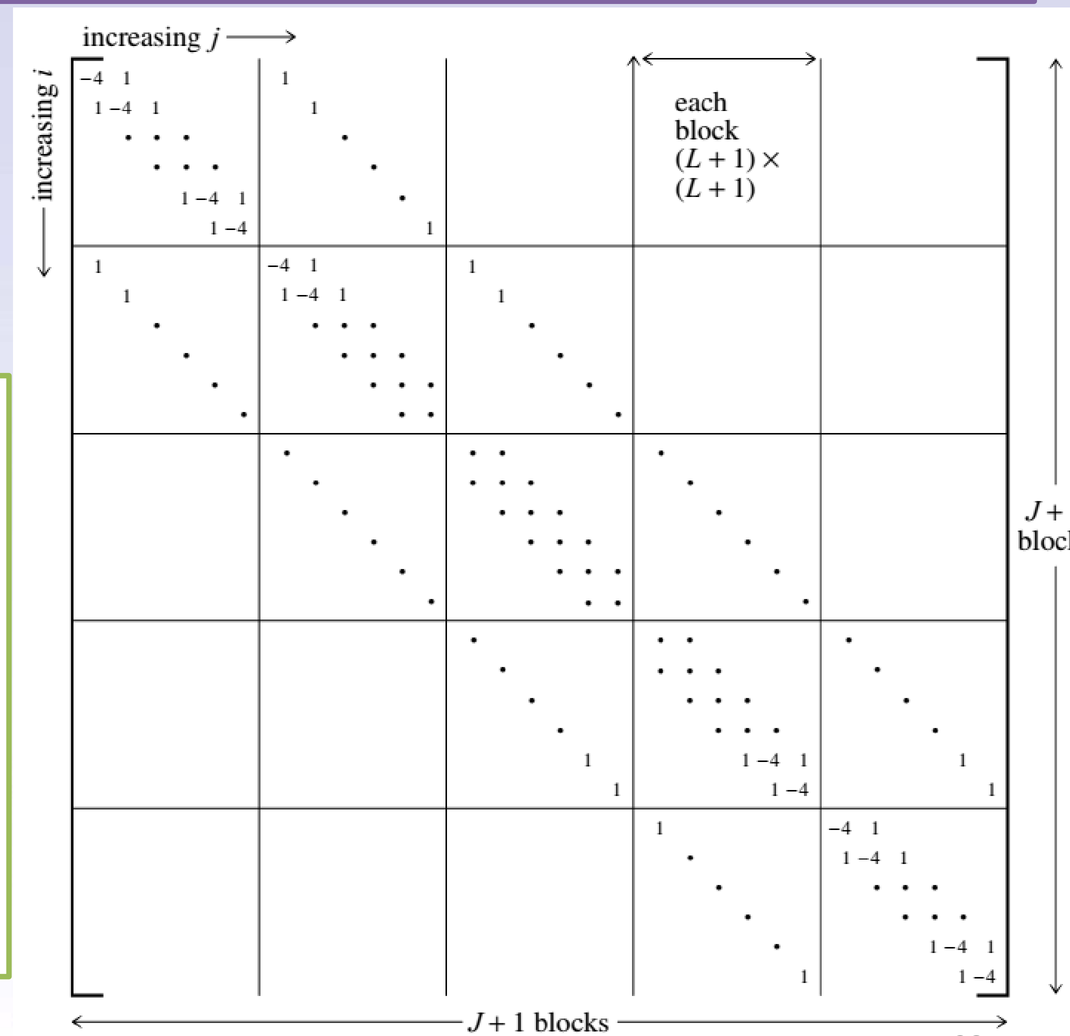
Finite Difference Method

FDM for Laplace equation – form a system of linear equations

$$AU = b$$

$$\begin{bmatrix} -4 & 1 & 1 & 0 \\ 1 & -4 & 0 & 1 \\ 1 & 0 & -4 & 1 \\ 0 & 1 & 1 & -4 \end{bmatrix} \begin{bmatrix} U_{1,1} \\ U_{2,1} \\ U_{1,2} \\ U_{2,2} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}$$

- **b contains boundary information**
- **A is block tridiagonal**
- **Structure of A depends on the order of grid points**
- **Can be solved using iterative or direct methods, such as Gaussian elimination**



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FEM

Finite Element Method

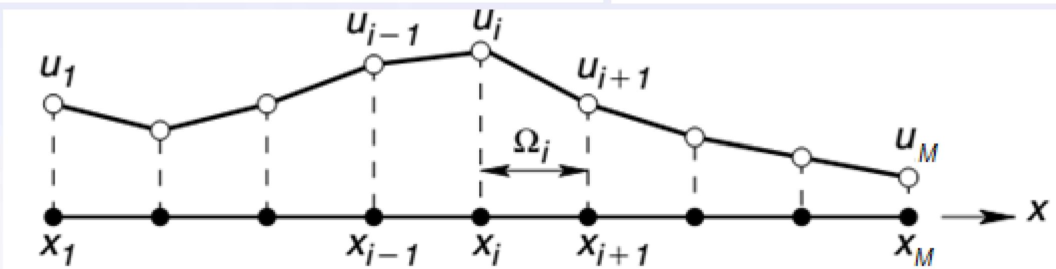
Features

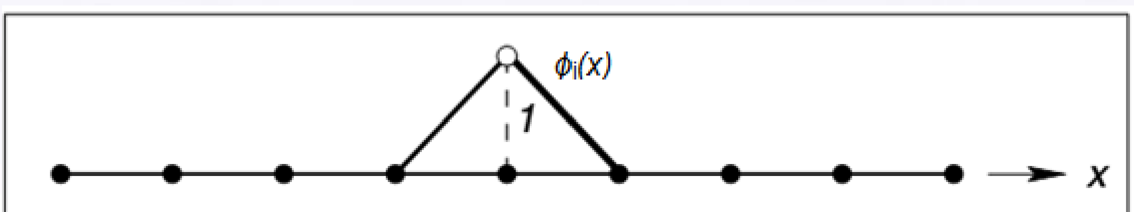
- Complicated geometries
- High-order approximations
- Strong mathematical foundation
- Flexibility

Basic Idea

$$u(\mathbf{x}) \approx \hat{u}(\mathbf{x}) = \sum_{j=1}^{M} u_j \phi_j(\mathbf{x})$$

- ϕ_j are basis functions
- u_j: M unknowns; Need M equations
- Discretizing derivatives results in linear system





Finite Element Method

Poisson's Equation – Elliptic

$$-\Delta u(x) = f(x)$$

$$\Delta = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Steady state heat transfer

$$\underbrace{kA\frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}}_{\text{Heat conduction}} \underbrace{-hP\phi + hP\phi_f}_{\text{Heat convection}} + \underbrace{q}_{\text{Heat supply}} = 0$$

1D Example

$$-u'' = f, \qquad 0 < x < 1$$

$$u(0) = u(1) = 0$$

- Solution must be twice differentiable
- Unnecessarily strong if *f* (e.g., heat supply) is discontinuous

Finite Element Method

Weak Formulation

Multiply both sides by an arbitrary test function v and integrate

$$\int_0^1 -u''v\,dx = \int_0^1 fv\,dx$$

$$\int_0^1 u'v'\,dx - u'v|_0^1 = \int_0^1 fv\,dx.$$

$$\int_0^1 u'v'\,dx = \int_0^1 fv\,dx.$$

Since v was arbitrary, this equation must hold for all v such that the equation makes sense (v' is square integrable), and $v(0) = v(1) = 0$.

Finite Element Method

- Approximation

$$\int_0^1 u'v'dx = \int_0^1 fvdx.$$

$$u(\mathbf{x}) \approx \hat{u}(\mathbf{x}) = \sum_{i=1}^{M} \xi_i \phi_i(x)$$

The Basic Idea of FEM

$$\int_0^1 \hat{u}'\hat{v}'dx = \int_0^1 f\hat{v}dx \quad \xrightarrow{\hat{v}=\phi_i(x)} \quad \int_0^1 \sum_{i=1}^{M} \xi_i \phi_i' \phi_j' dx = \int_0^1 f\phi_j dx$$

Thus if $A = (a_{ij})$ with $a_{ij} = \int_0^1 \phi_i'\phi_j' dx$ and $b = (b_i)$ with $b_i = \int_0^1 f\phi_i dx$, then

$$A\xi = b$$

Linear System of Equations

Finite Element Method

- Basis functions

we are looking for functions with the following property

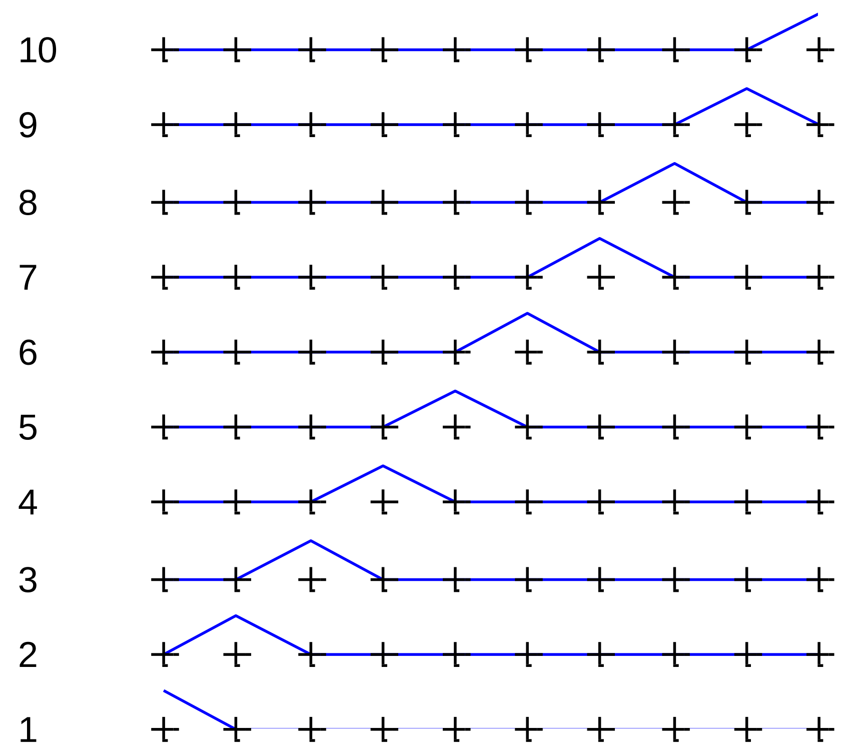
$$\phi_i(x) = \begin{cases} 1 & for \quad x = x_i \\ 0 & for \quad x = x_j,\ j \neq i \end{cases}$$

... otherwise we are free to choose any function ...

The simplest choice are of course linear functions:

+ grid nodes

blue lines – basis functions φ_i



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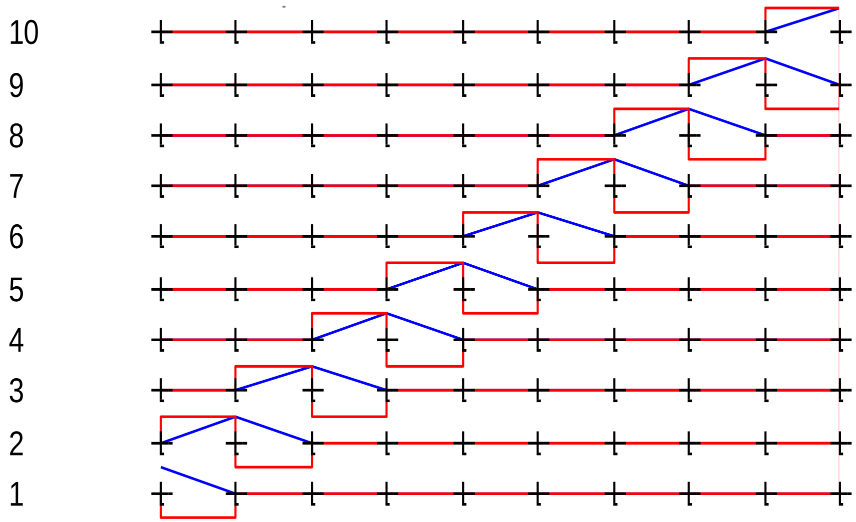
Finite Element Method

Stiffness Matrix

$$A = (a_{ij}) \text{ with } a_{ij} = \int_0^1 \phi_i' \phi_j' dx$$



To assemble the stiffness matrix we need the gradient (red) of the basis functions (blue)

For the special case when $h_j \equiv h$ we have

$$\frac{1}{h}\begin{bmatrix} 2 & -1 & 0 & \cdots & \cdots & 0 \\ -1 & 2 & -1 & \ddots & & \vdots \\ 0 & -1 & 2 & -1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & -1 & 2 & -1 \\ 0 & \cdots & \cdots & 0 & -1 & 2 \end{bmatrix}$$

Finite Element Method

- Compare to FDM

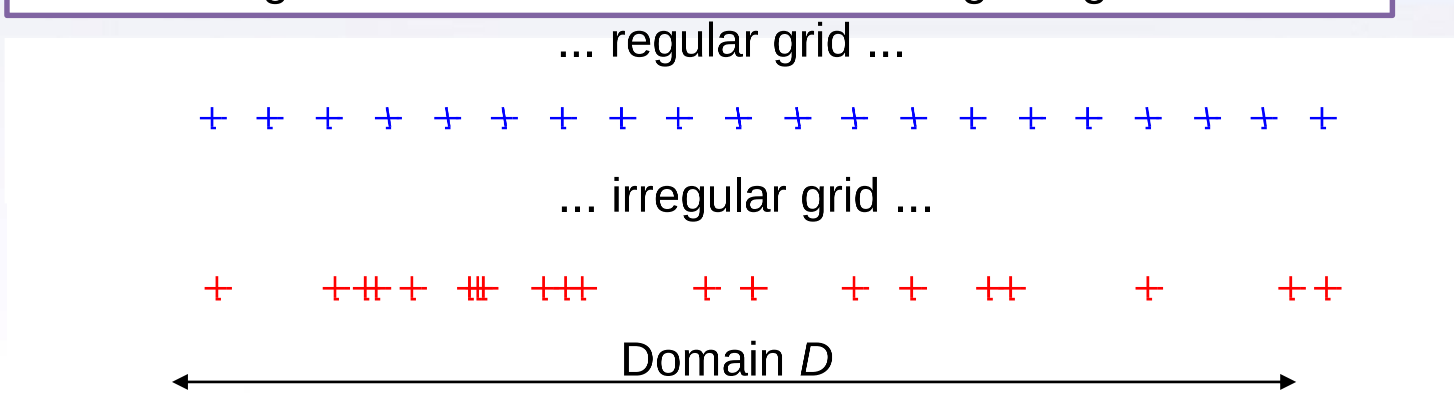
$$b = (b_i) \text{ with } b_i = \int_0^1 f\phi_i dx$$

Note that if Trapezoid rule is used to approximate the right hand side, then $b_i = hf_i$, and therefore the equations determining $\hat{u}$ are

$$\frac{\xi_{i+1} - 2\xi_i + \xi_{i-1}}{h} = hf_i$$

which are exactly the same as FDM.

- Advantage of FEM: do not have to use regular grid



Finite Element Method

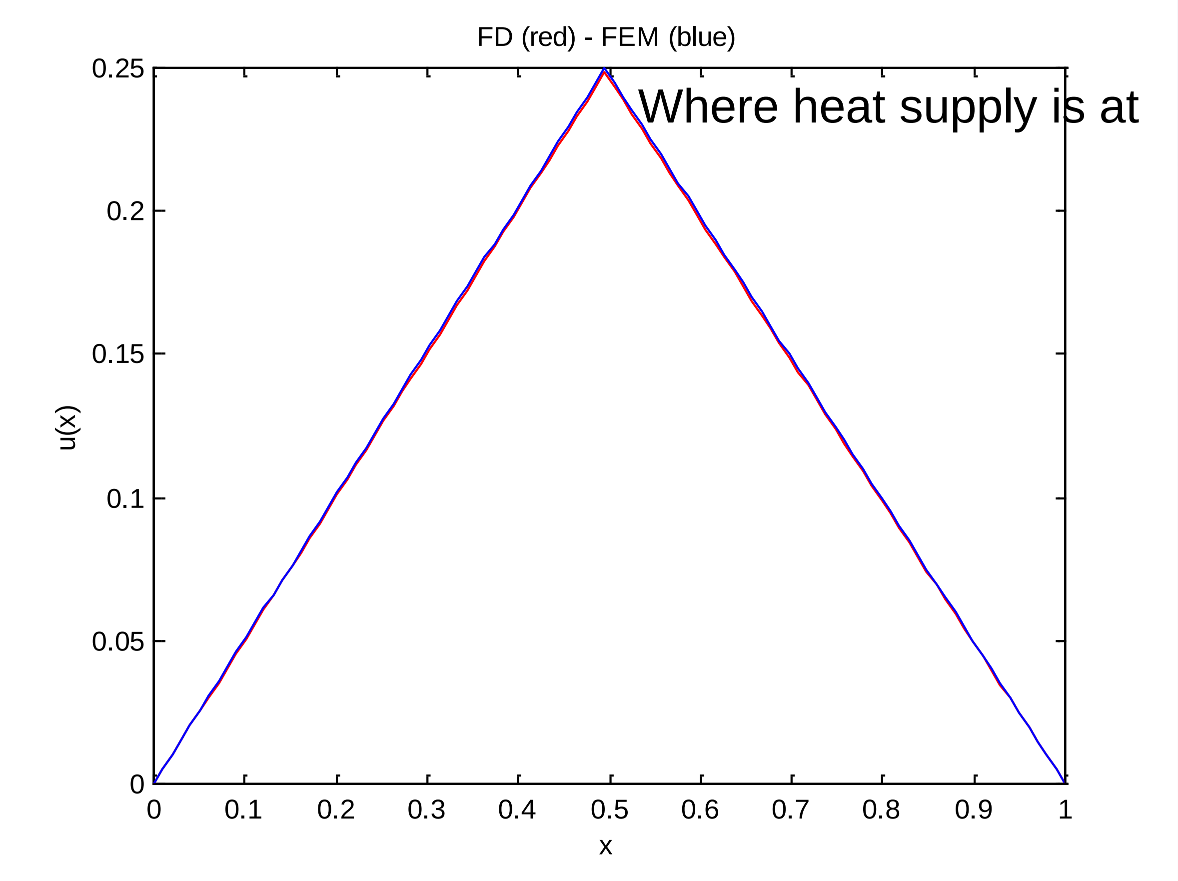
- Simplest Matlab FEM code

```
% source term
b=(1:nx)*0;b(nx/2)=1.;
% boundary left  u_1  int{ nabla phi_1  nabla phij }
u1=0;   b(1) =0;
% boundary right  u_nx int{ nabla phi_nx nabla phij }
unx=0; b(nx)=0;

% assemble matrix Aij

A=zeros(nx);

for i=2:nx-1,
   for j=2:nx-1,
      if i==j,
         A(i,j)=2/dx;
      elseif j==i+1
         A(i,j)=-1/dx;
      elseif j==i-1
         A(i,j)=-1/dx;
      else
         A(i,j)=0;
      end
   end
End
% solve linear system of equations
fem(2:nx-1)=inv(A(2:nx-1,2:nx-1))*s(2:nx-1)'; fem(1)=u1;
fem(nx)=unx;
```

Domain: [0,1]; nx=100;
dx=1/(nx-1);f(x)=d(1/2)
Boundary conditions:
u(0)=u(1)=0

Finite Element Method

- Results



Solving Linear Systems

- Equations

$$
\begin{aligned}
10x_1 - 7x_2 &= 7, \\
-3x_1 + 2x_2 + 6x_3 &= 4, \\
5x_1 - x_2 + 5x_3 &= 6.
\end{aligned}
$$

- Matrix form

$$
\begin{pmatrix} 10 & -7 & 0 \\ -3 & 2 & 6 \\ 5 & -1 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 4 \\ 6 \end{pmatrix}
$$

- In Matlab

$X = A\backslash B.$ Or $X = A^{-1}B$

Solving Linear Systems

- Linear Algebra (Solving Linear Algebraic Equations)

- Direct(LU factorization)
  - More accurate
  - Maybe cheaper for many time steps
  - Banded matrix
  - Need more memory
  - Typically faster
- Iterative
  - Matrix-free (less memory)
  - Sparse
  - SPD (Symmetric Positive Definite)
  - Converging Issue


THANK
YOU!