Finite Difference, Finite Element and Finite Volume Methods for the Numerical Solution of PDEs

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DOE Multiscale Summer School

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Math Modeling and Simulation of Physical Processes

- Define the physical problem

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- Create a mathematical (PDE) model
  - Systems of PDEs, ODEs, algebraic equations
  - Define Initial and or boundary conditions to get a well-posed problem

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- Analyse Errors in the discrete system
  - Consistency, stability and convergence analysis

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- Partial Differential Equations (PDEs)

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- Iterative Methods for large sparse linear systems

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- Boundary conditions, i.e., conditions on the (finite) boundary of the domain ann/or initial conditions (for transient problems) are required to obtain a *well posed problem*.

PDEs (continued)

- For simplicity, we will deal only with single PDEs (as opposed to systems of several PDEs) with only two independent variables,
  - either two space variables, denoted by x and y, or
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- For simplicity, we will deal only with single PDEs (as opposed to systems of several PDEs) with only two independent variables,
  - either two space variables, denoted by x and y, or
  - one space variable denoted by x and one time variable denoted by t
- Partial derivatives with respect to independent variables are denoted by subscripts, for example
  - $u_t = \frac{\partial u}{\partial t}$
  - $u_{xy} = \frac{\partial^2 u}{\partial x \partial y}$

Well Posed Problems

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- Properties of a well posed problem:
  - Solution exists
  - Solution is unique
  - Solution depends continuously on the data

Classifications of PDEs

- The Order of a PDE = the highest-order partial derivative appearing in it. For example,
  - The advection equation $u_t + u_x = 0$ is a first order PDE.
  - The Heat equation $u_t = u_{xx}$ is a second order PDE.

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- A PDE is linear if the coefficients of the partial derivates are not functions of u, for example
  - The advection equation $u_t + u_x = 0$ is a linear PDE.
  - The Burgers equation $u_t + u u_x = 0$ is a nonlinear PDE.

Classifications of PDEs (continued)

Second-order linear PDEs of general form

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

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.

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- $b^2 - 4ac < 0$: elliptic
    - e.g., Laplace equation: $u_{xx} + u_{yy} = 0$
    - Elliptic PDEs describe processes that have alreay reached steady states, and hence are time-independent.

Parabolic PDEs: Initial-Boundary value problems

- Example: One dimensional (in space) Heat Equation for $u = u(t, x)$

$$u_t = \kappa u_{xx}, \ 0 \leq x \leq L, \ t \geq 0$$

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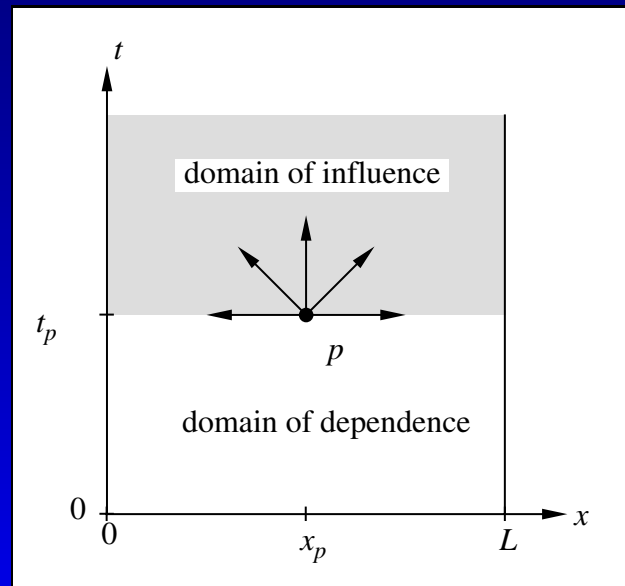
$$u_t = \kappa u_{xx}, \ 0 \le x \le L, \ t \ge 0$$

- with

  - Boundary conditions: $u(t, 0) = u_0, \ u(t, L) = u_L$, and

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  - $T(x, 0) = T_1, \ T(x, H) = T_3$
  - $T(0, y) = T_4, \ T(W, y) = T_2$

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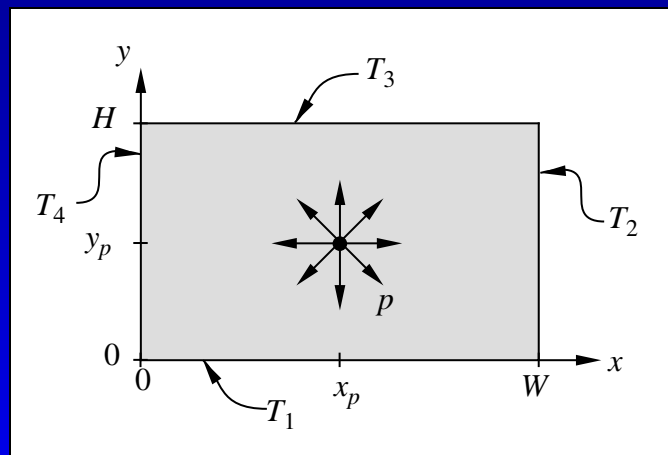
Hyperbolic PDEs: Initial-Boundary value problems

- Example: One-dimensional (in space) wave equation for $u = u(t, x)$

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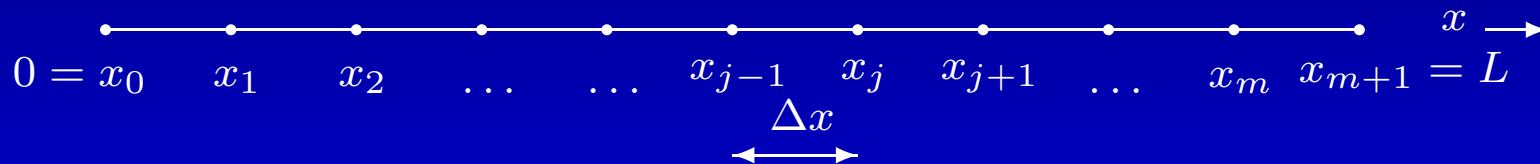 - Initial Conditions $u(0, x) = f(x), \ u_t|_{t=0} = g(x)$

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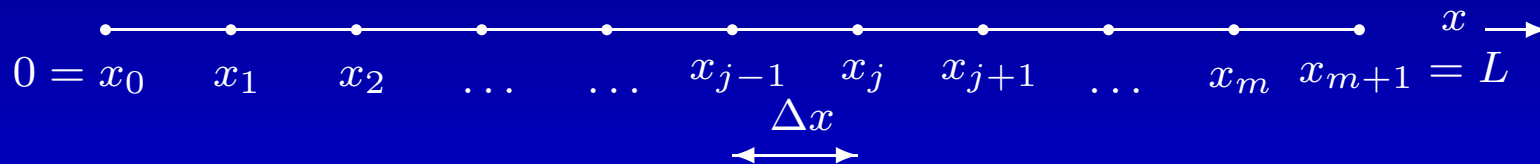
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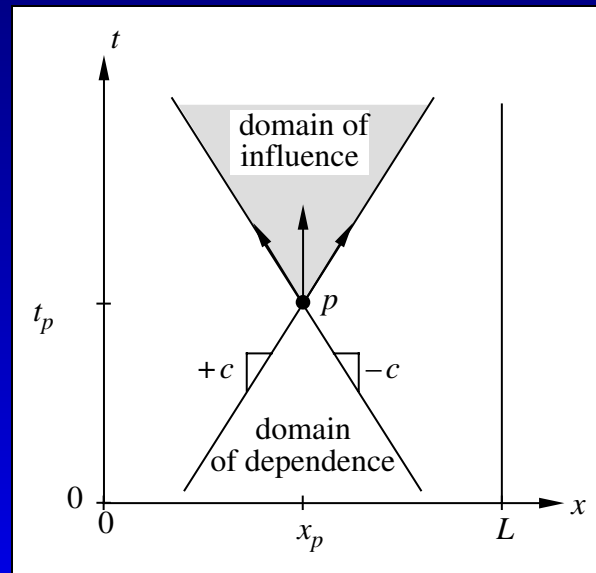
Finite Difference Methods (FDM): Discretization

- Suppose that we are solving for $u = u(t, x)$ on the domain $\Omega = [0, T] \times [0, L]$. we discretize the domain Ω by partitioning the spatial interval $[0, L]$ into $m + 2$ grid points $x_0, x_1, \ldots, x_m, x_{m+1} = L$, such that

$$\Delta x_j = x_{j+1} - x_j, j = 0, 1, 2, \ldots m$$

In the case that the $m + 2$ spatial points x_j are equally spaced, we have

$$\Delta x = \Delta x_j, \forall j$$

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- We similarly discretize the temporal domain $[0,T]$ into discrete time levels t_k with time step $k = \Delta t$.

Finite Difference Methods: Discretization

- The numerical solution to the PDE is an approximation to the exact solution that is obtained using a discrete represntation to the PDE at the grid points x_j in the discrete spatial mesh at every time level t_k. Let us denote this numerical solution as U such that

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- The boundary conditions determine the values of U_0^n and U_{m+1}^n for all n. The initial conditions determine the values of U^0 at each spatial grid point.

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Finite Difference Methods (continued)

- Recall the definition of the derivative from introductory Calculus:

$$u_x(x_j) = \lim_{h \to 0} \frac{u(x_j + h) - u(x_j)}{h}$$

$$= \lim_{h \to 0} \frac{u(x_j) - u(x_j - h)}{h}$$

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

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- We use these formula with a small finite value of $h = \Delta x$, i.e., we approximate

$$u_x(x_j) \approx \frac{u(x_j + h) - u(x_j)}{h} \ (\text{Forward difference})$$

$$\approx \frac{u(x_j) - u(x_j - h)}{h} \ (\text{Backward difference})$$

$$\approx \frac{u(x_j + h) - u(x_j - h)}{2h} \ (\text{Centered difference})$$

Error in FDM: Local Truncation Error

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$$u(x_{j+1}) = u(x_j + \Delta x)$$

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$$u_x(x_j) = \frac{u(x_{j+1}) - u(x_j)}{\Delta x} + u_{xx}(x_j)\frac{\Delta x}{2} + O((\Delta x)^2)$$

- The forward difference is a first order accurate approximation to the partial derivative u_x at x_j and the LTE is $O(\Delta x)$.

Error in FDM: LTE

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- The centered difference is a second order accurate approximation to the partial derivative u_x at x_j and the LTE is $O((\Delta x)^2)$.

- Note that the LTE in all these approximations goes to zero as Δx goes to zero.

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FDM for Parabolic PDEs: The Heat Equation

- Consider the initial-boundary value problem for the heat equation
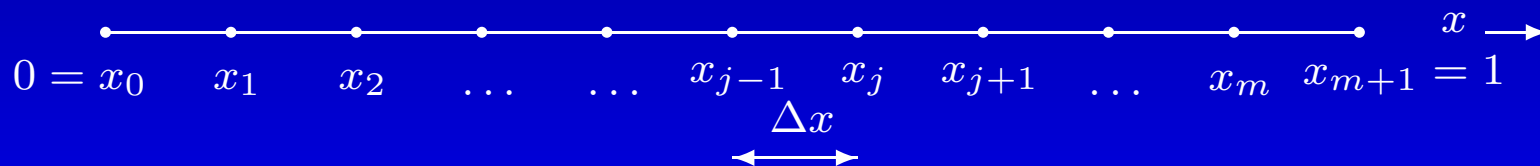
$$u_t = \kappa u_{xx}, \ 0 \le x \le 1, \ t \ge 0$$

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

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

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

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- 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 $x_j, j = 0, 1, \ldots m + 1$.

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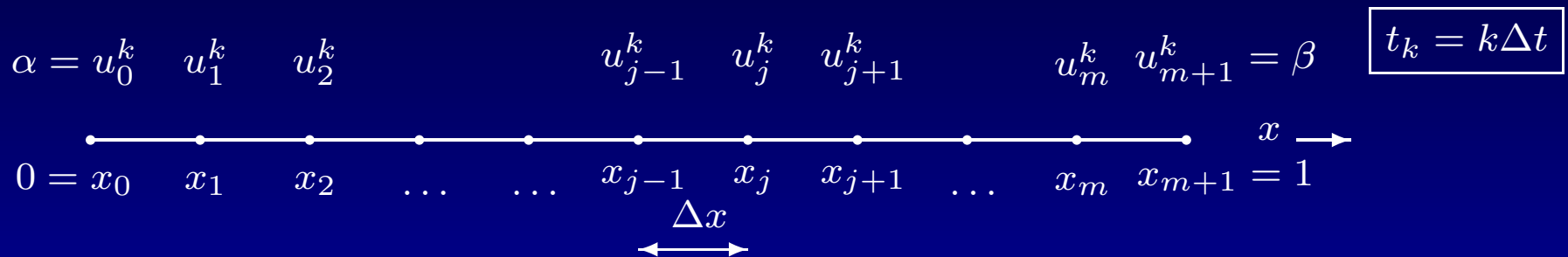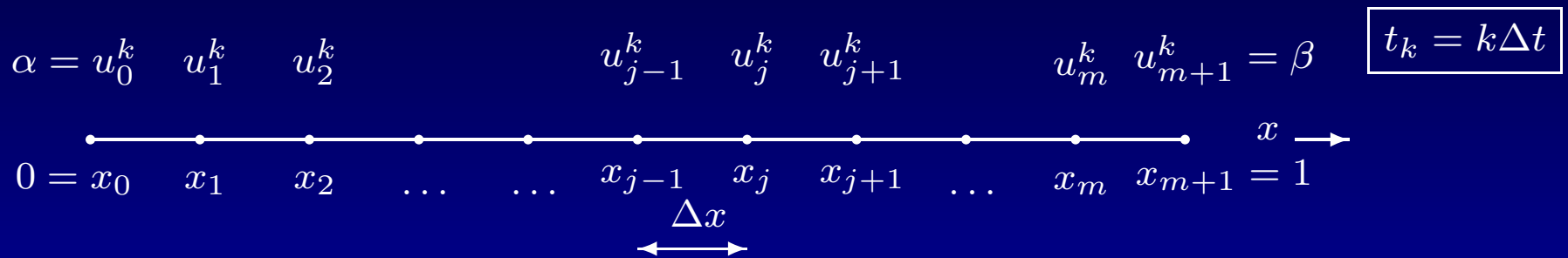# FDM for Parabolic PDEs: The Heat Equation

- Similarly discretize the temporal domain into temporal grid points $t_k = k\Delta t$ for suitably chosen time step Δt.
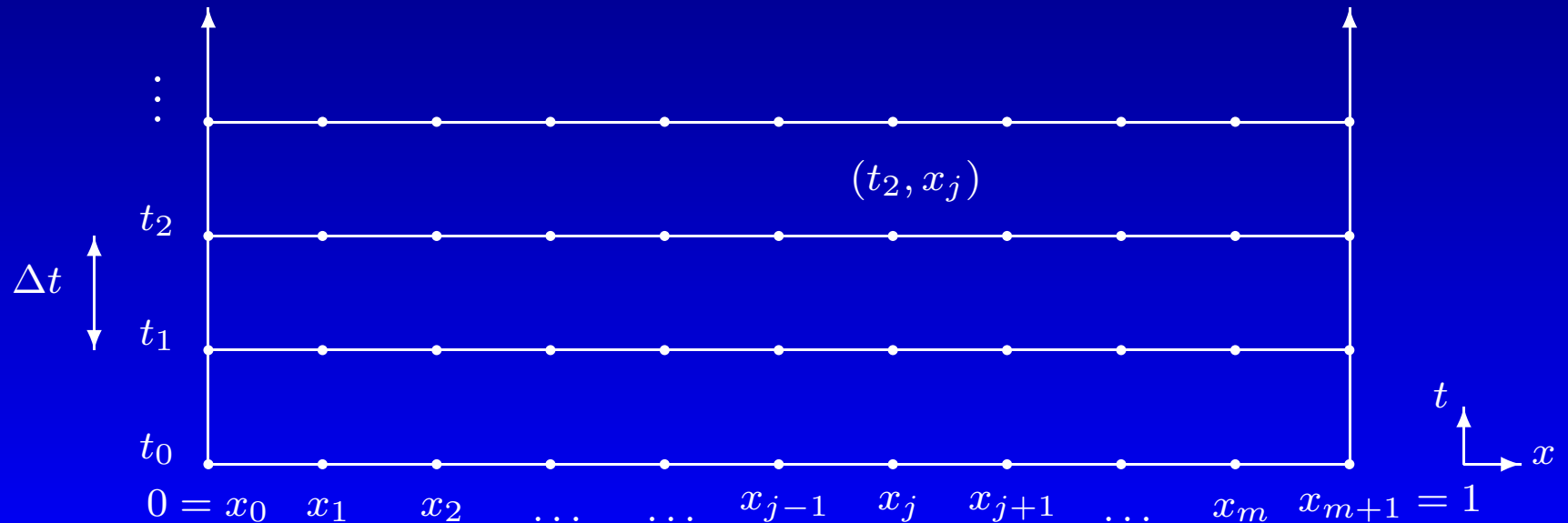
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- Denote the approximate solution at the grid point (t_k, x_j) as U_j^k.

$$\alpha = u_0^k \quad u_1^k \quad u_2^k \qquad\qquad u_{j-1}^k \quad u_j^k \quad u_{j+1}^k \qquad\qquad u_m^k \quad u_{m+1}^k = \beta$$

$$\boxed{t_k = k\Delta t}$$

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$$\Delta x$$

$$x$$

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Δx

- The space-time grid can be represented as

(t_2, x_j)

t_2

Δt

t_1

t_0

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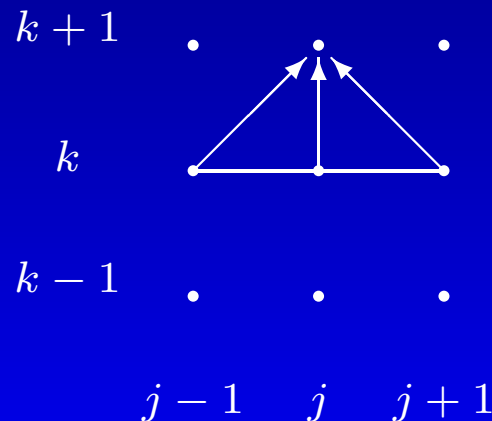
FDM for Parabolic PDEs: The Heat Equation

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

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

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

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- Associated to this scheme is a Computational Stencil

$k + 1$

k

$k - 1$

$j - 1 \quad j \quad j + 1$

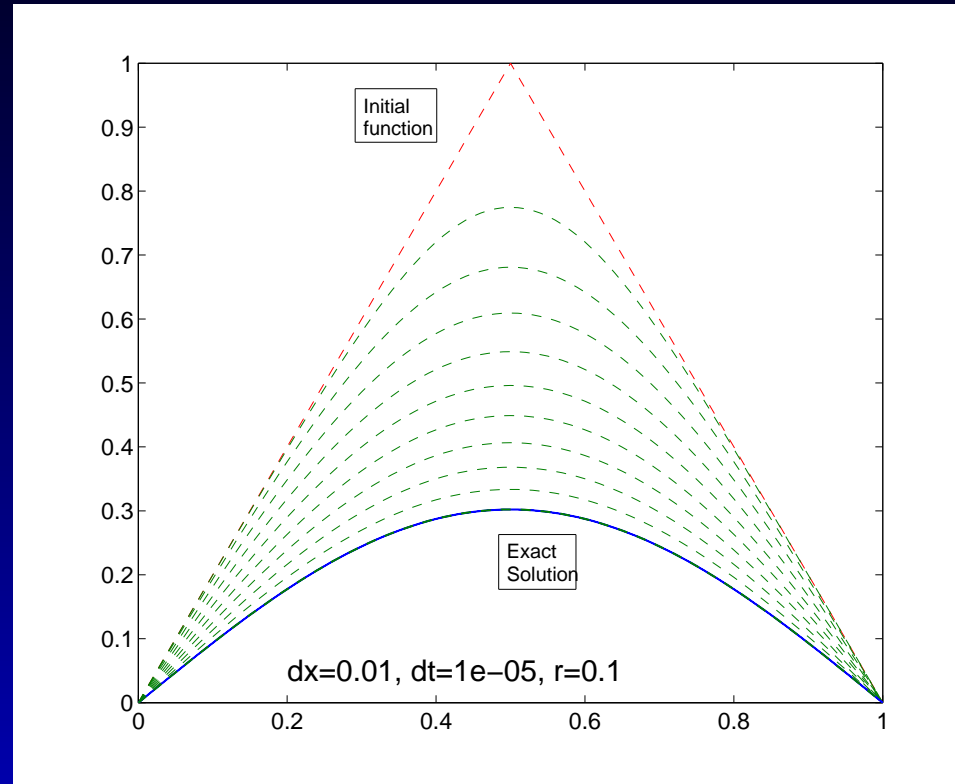OSU Oregon State University

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- We note that
  - From Boundary conditions: $U_0^k = \alpha$ and $U_{m+1}^k = \beta$ for all values of k.
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- The local truncation error is $O(\Delta t) + O((\Delta x)^2)$.

  Scheme is first order accurate in time and second order accurate in space

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FDM for Parabolic PDEs: The Heat Equation

- This is an explicit FDM for the heat equation: Solution at time level $k+1$ is determined by solution at previous time levels only.

- We note that
  - From Boundary conditions: $U_0^k = \alpha$ and $U_{m+1}^k = \beta$ for all values of k.
  - From Initial condition: $U_j^0 = f(x_j)$ for all values of j.

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

  Scheme is first order accurate in time and second order accurate in space

- How do we choose the values of Δt and Δx??

FDM for Parabolic PDEs: The Heat Equation

- Initial condition has a discontinuous derivative at $x = 0.5$.

FDM for Parabolic PDEs: The Heat Equation

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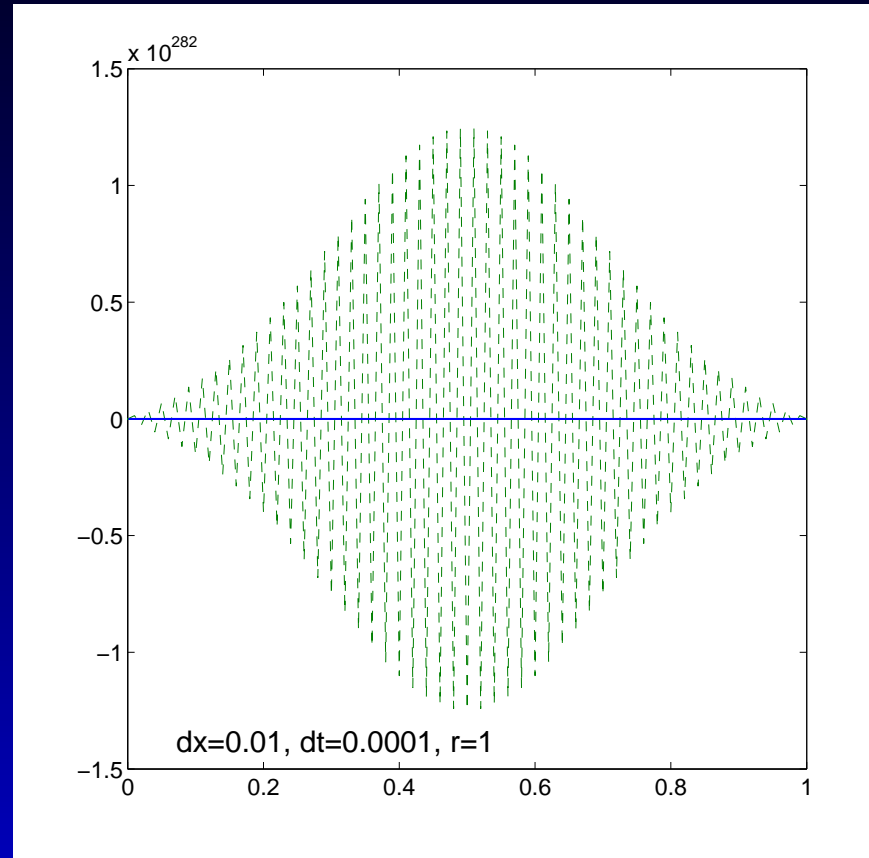# FDM for Parabolic PDEs: The Heat Equation

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- However, we see a rapid smoothing effect of this initial discontinuity as time evolves.

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

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

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- What happens if this value is greater than 1/2?

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FDM for Parabolic PDEs: The Heat Equation
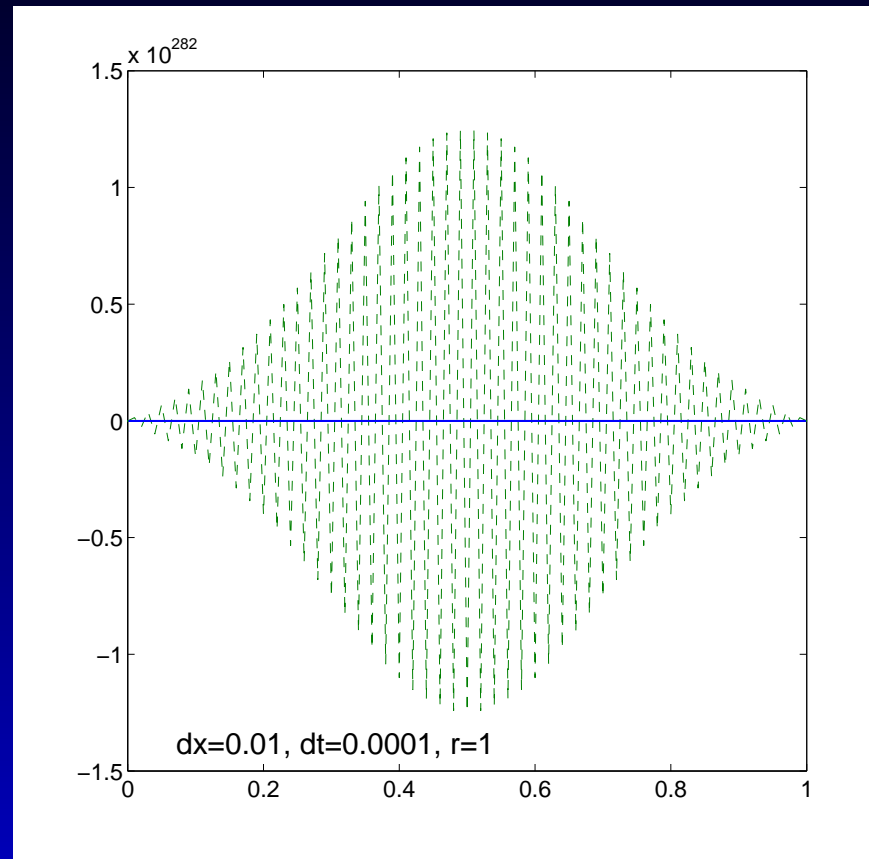
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- Thus, Δt and Δx cannot be chosen arbitrarily. They have to satisfy a stability condition.

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Implicit FDM for Parabolic PDEs: The Heat Equation

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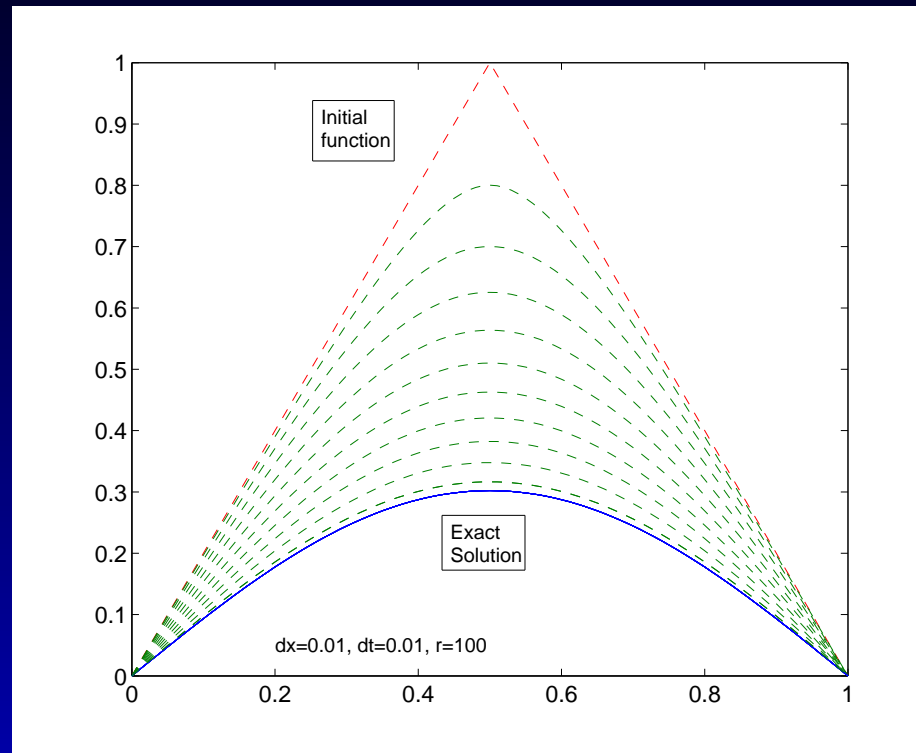
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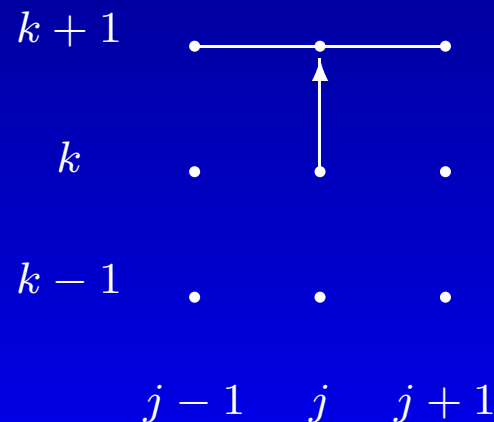
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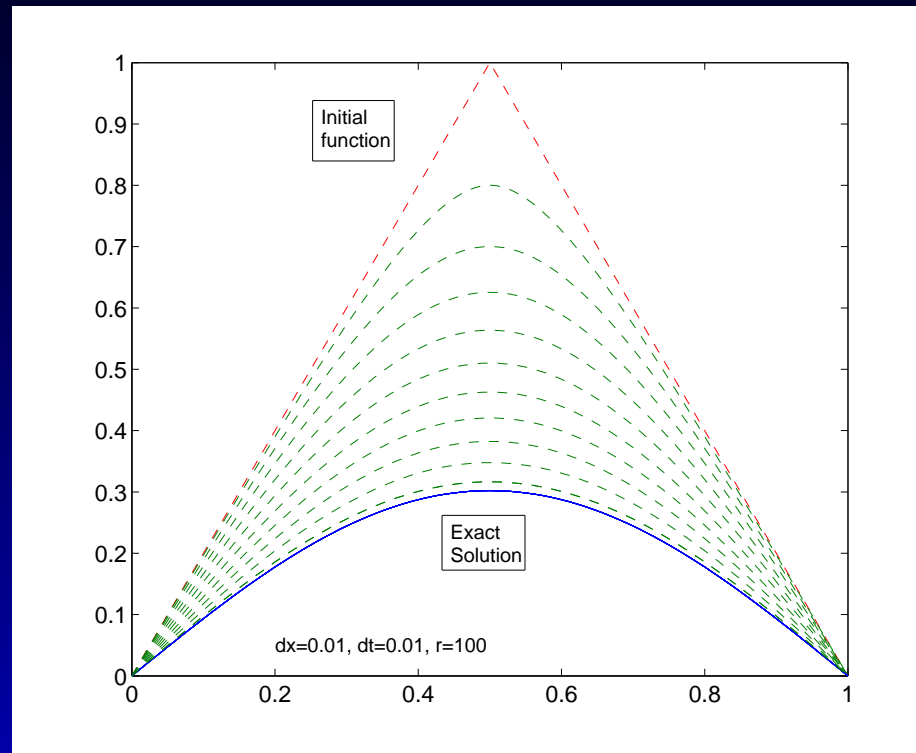
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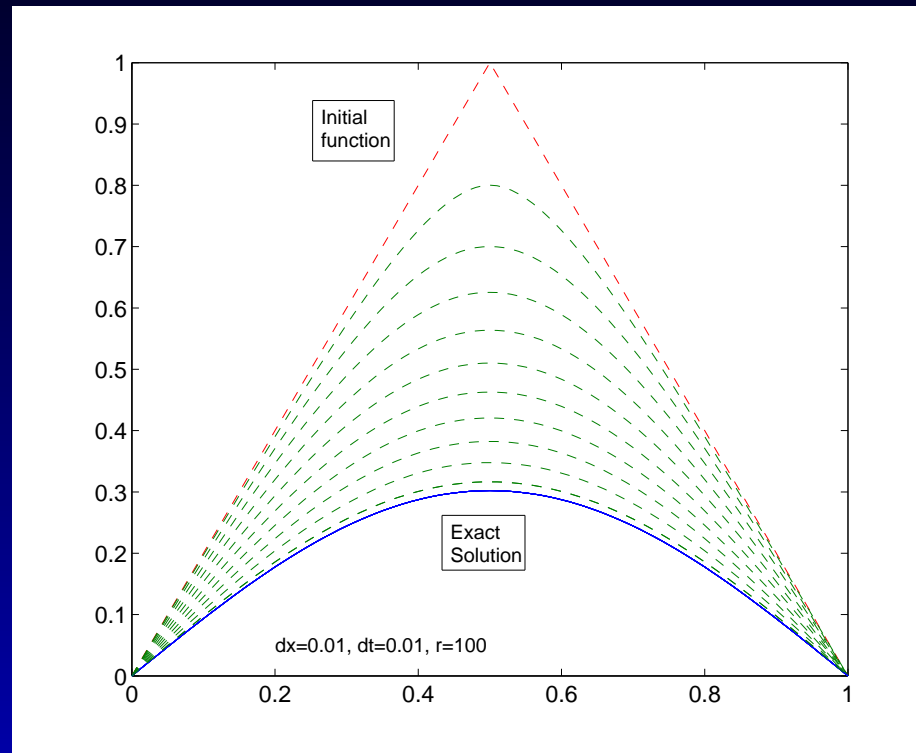
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- The implicit FDM is unconditionally stable

Crank-Nicolson for The Heat Equation

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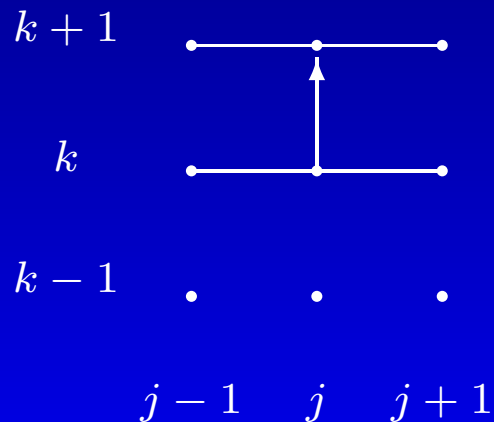
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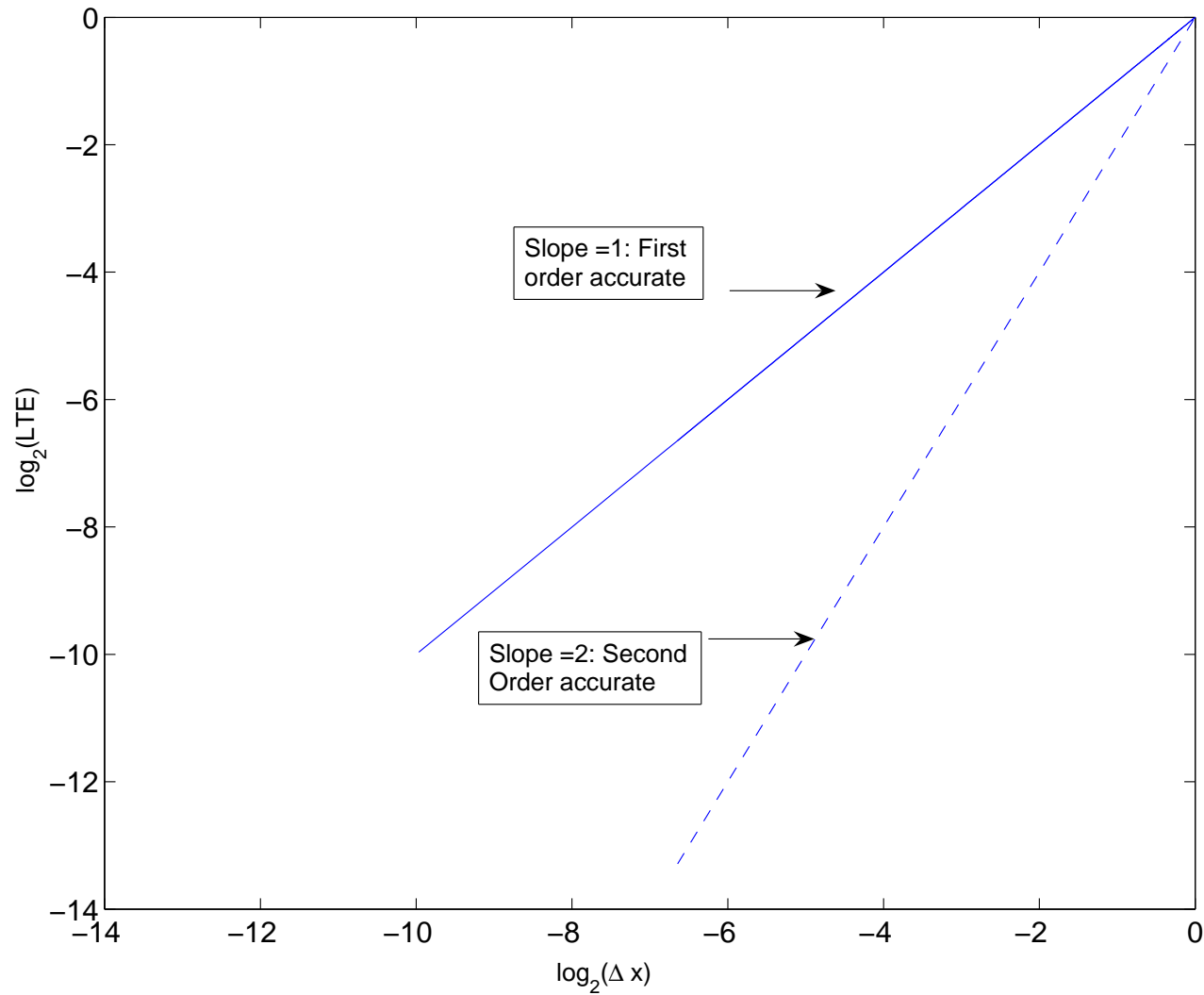
$$j = 1, 2, \ldots m$$

- Associated to this scheme is a Computational Stencil

- This method is unconditionally stable,

- and second-order accurate in time

- However a system of equations must be solved at each time step.

First vs Second Order Accuracy

Method of Lines (MOL) Discretization

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- The method of lines approach can be used to analyze the stability of the numerical method for the PDE by analyzing the eigenvalues of the matrix of the resulting system of ODEs using the ideas of absolute stability for ODEs.

Analysis of FDM

- Consitency implies that the local truncation error goes to zero as Δx and Δt approach zero. This is usually proved by invoking Taylor's theorem.

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  - Eigenvalue analysis of the matrix representation of the FDM.
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  - Eigenvalue analysis of the matrix representation of the FDM.
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  - Computing the domain of dependence of the numerical method.

- Lax-Equivalence Theorem : A consistent approximation to a well-posed problem is convergent if and only if it is stable

Von Neumann Analysis for Time-dependent Problems

- Example: The analytical solutions of the heat equation $u_t - \kappa u_{xx} = 0$ can be found in the form

$$u(t, x) = \sum_{-\infty}^{\infty} e^{\beta_m t} e^{i\alpha_m x}$$

with $\beta_m + \kappa \alpha_m^2 = 0$. Here $e^{i\alpha_m x} = \cos(\alpha_m x) + i \sin(\alpha_m x)$.

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- Thus requiring that this amplification factor G is bounded by one as $k \to \infty$ gives rise to a relation between Δt and Δx called the von Neumann stability condition.

FDM for Hyperbolic PDEs: The Advection Equation

- Consider the initial value problem for the Advection equation

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

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

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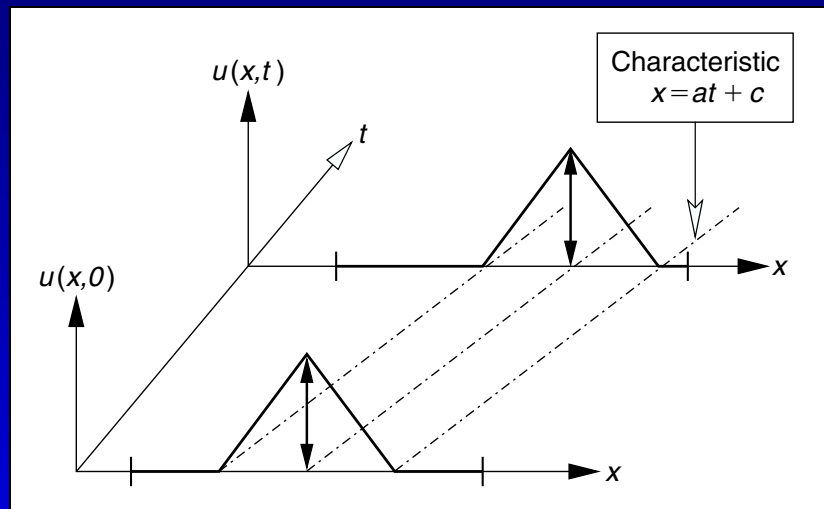- The solution $u(x,t) = f(x - at)$ is a wave that propagates to the right if $a > 0$ and to the left if $a < 0$.

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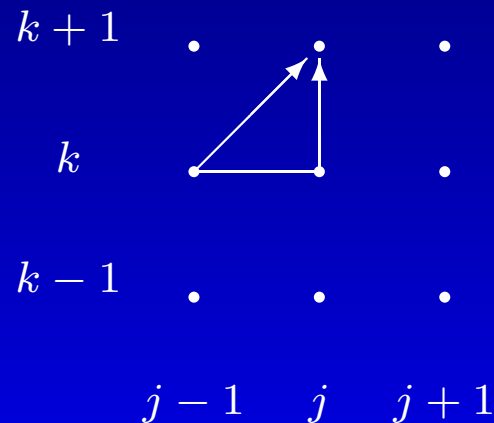
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$$\frac{U_j^{k+1} - U_j^k}{\Delta t} + a \frac{U_{j+1}^k - U_j^k}{\Delta x} = 0$$

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

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- Associated to this scheme is a Computational Stencil

  $k+1$

  k

  $k-1$

  $j-1 \quad j \quad j+1$

  - Scheme is explicit

  - First order accurate is time and space

  - Δt and Δx are related through the Courant number
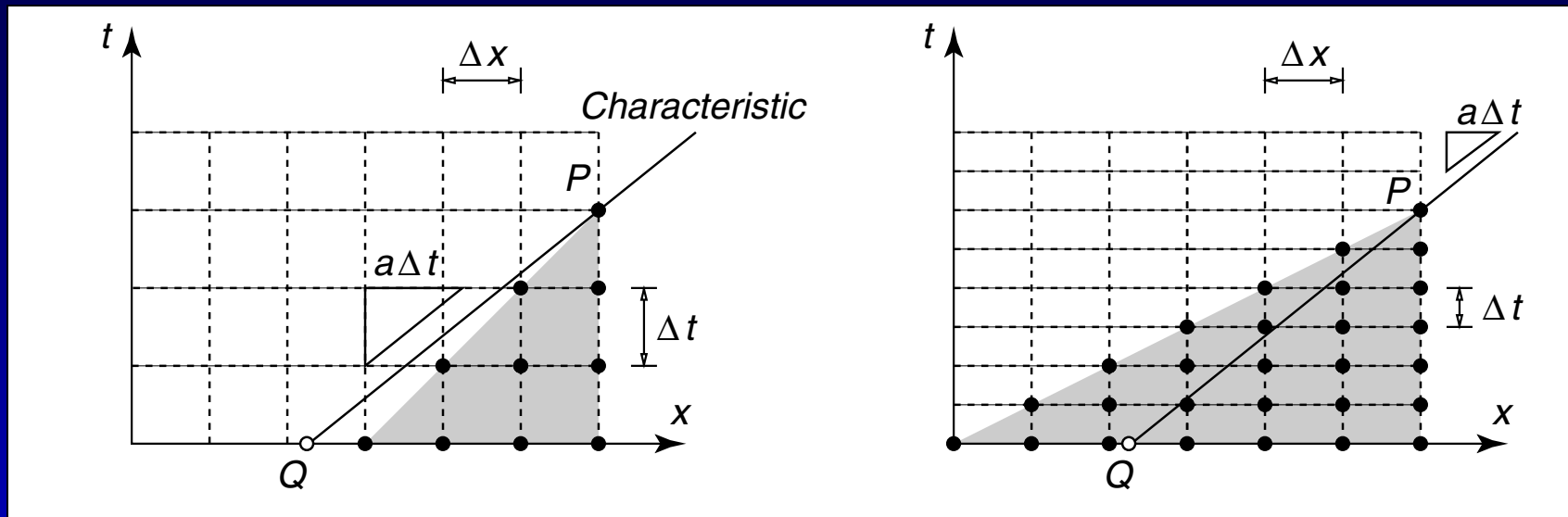 $$\nu = \frac{a\Delta t}{\Delta x}$$

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Courant Friedrich Lewy (CFL) Condition

- The CFL Condition : For stability, at each mesh point, the Domain of depencence of the PDE must lie within the domain of dependence of the numerical scheme.
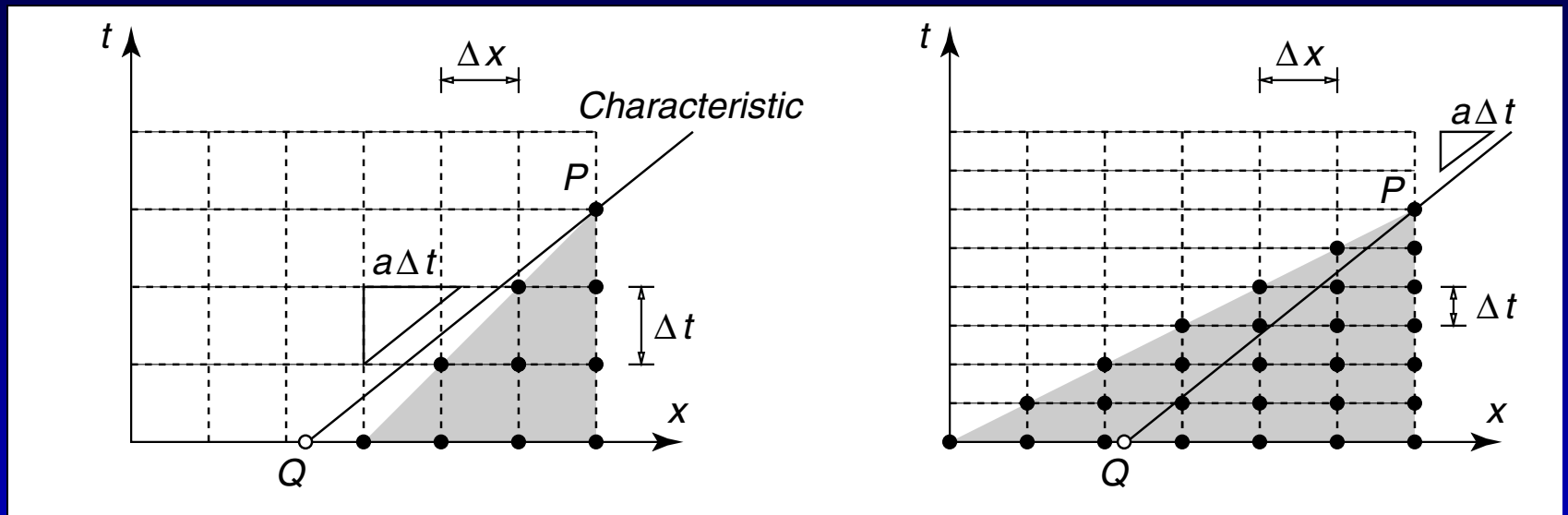
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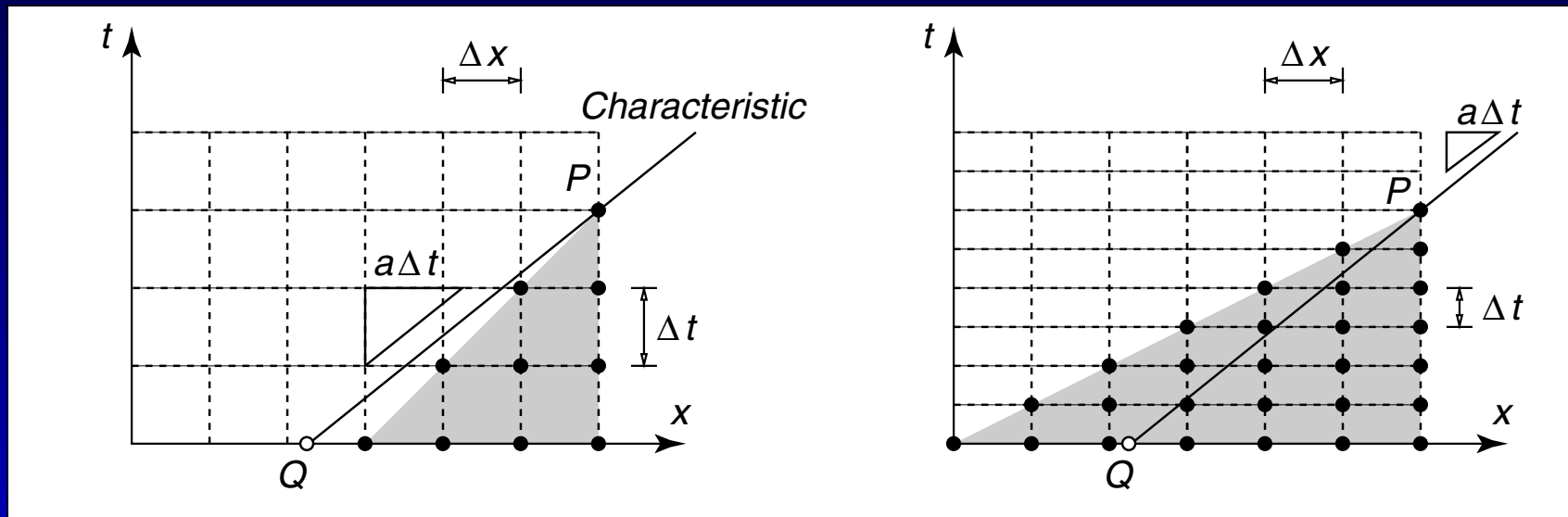
- CFL is a necessary condition for stability of explicit FDM applied to Hyperbolic PDEs. It is not a sufficient condition.

- For the advection equation CFL condition for stability is $|\nu| \le 1$. i.e.,
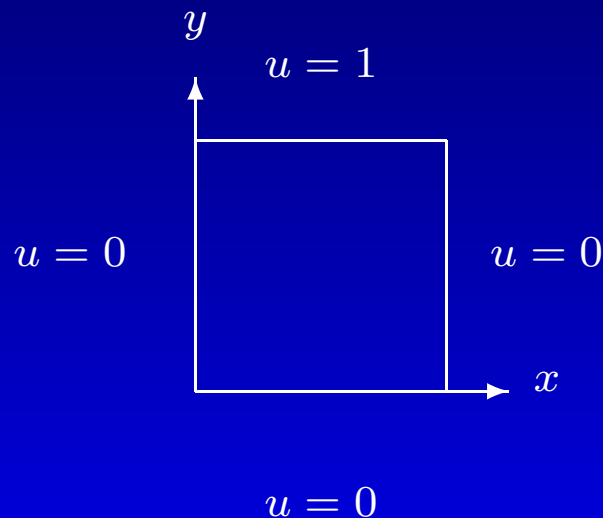$$\Delta t \le \frac{\Delta x}{|a|}.$$

Elliptic PDEs: Laplace Equation

- Time-independent problems

Elliptic PDEs: Laplace Equation

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- Consider the Boundary value problem for Laplace equation in two spatial dimensions
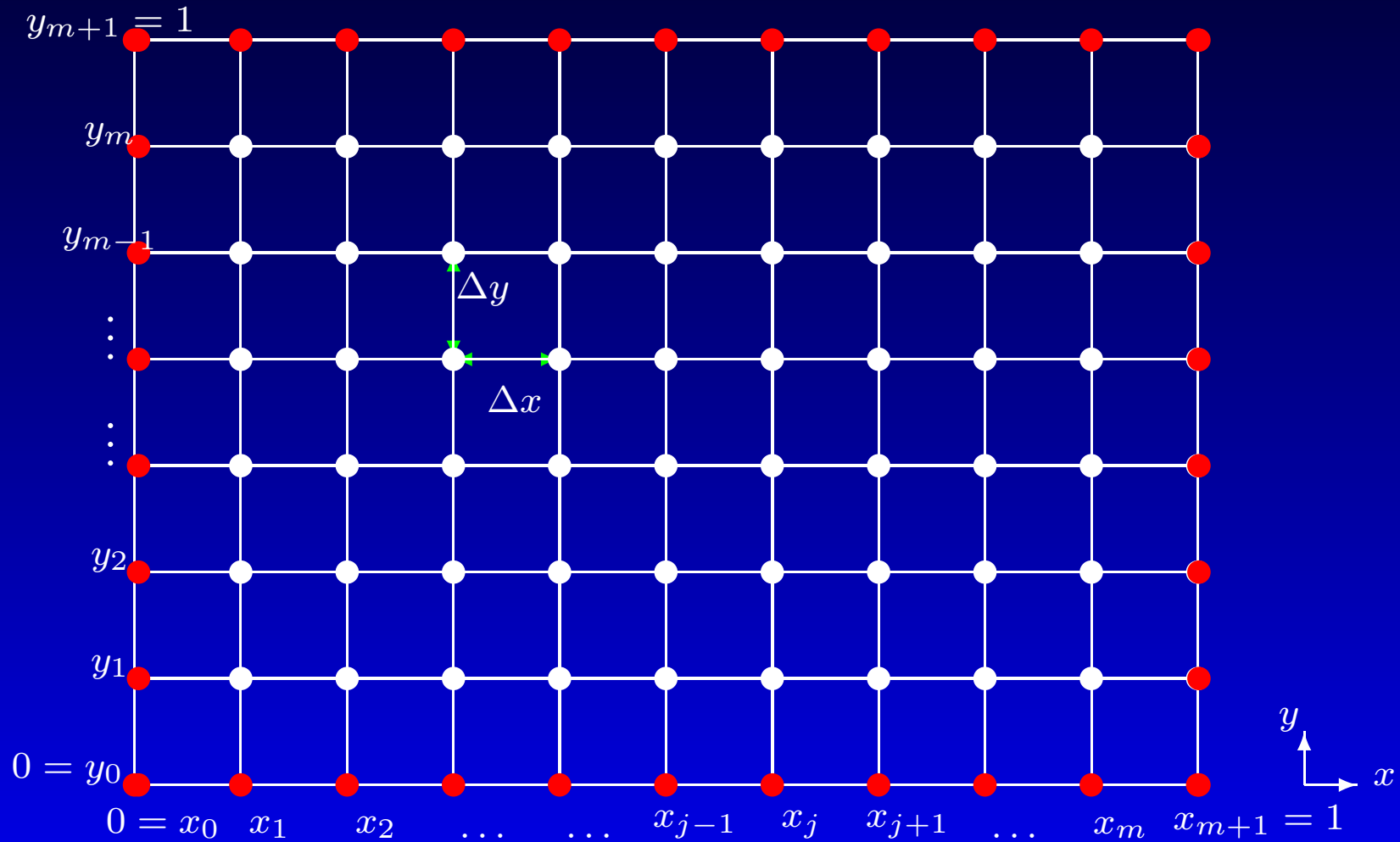
$$u_{xx} + u_{yy} = 0, \ 0 \le x \le 1, \ 0 \le y \le 1$$

with boundary conditions prescibed as shown below

FDM for Elliptic PDEs: Laplace Equation

- Discretize the mesh using uniform mesh step in both the x and y directions as below.

Elliptic PDEs: Laplace Equation

- Replace both the second order derivatives u_{xx} and u_{yy} with centered differences at each grid point (x_j, y_k) to obtain the difference scheme

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

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

$$U_{j+1,k} + U_{j-1,k} + U_{j,k+1} + U_{j,k-1} - 4U_{j,k} = 0$$
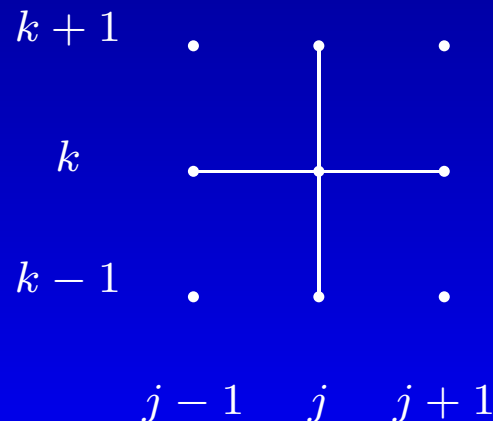
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- The Stencil for this FDM is called the Five-Point Stencil

Elliptic PDEs: Laplace Equation

- This FDM gives rise to a system of linear equations of the form

$$AU = b$$

- The right hand side vector b contains the boundary information.
- The vector U is the solution vector at the interior grid points.
- The matrix A is block tridiagonal if ordered in a *natural way*
- The structure of A depends on the ordering of the grid points.
- This system can be solved by iterative techniques or direct methods such as Gaussian elimination.

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- When $m = 2$, the system $AU = b$ can be written as

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

Discretization of Elliptic PDEs
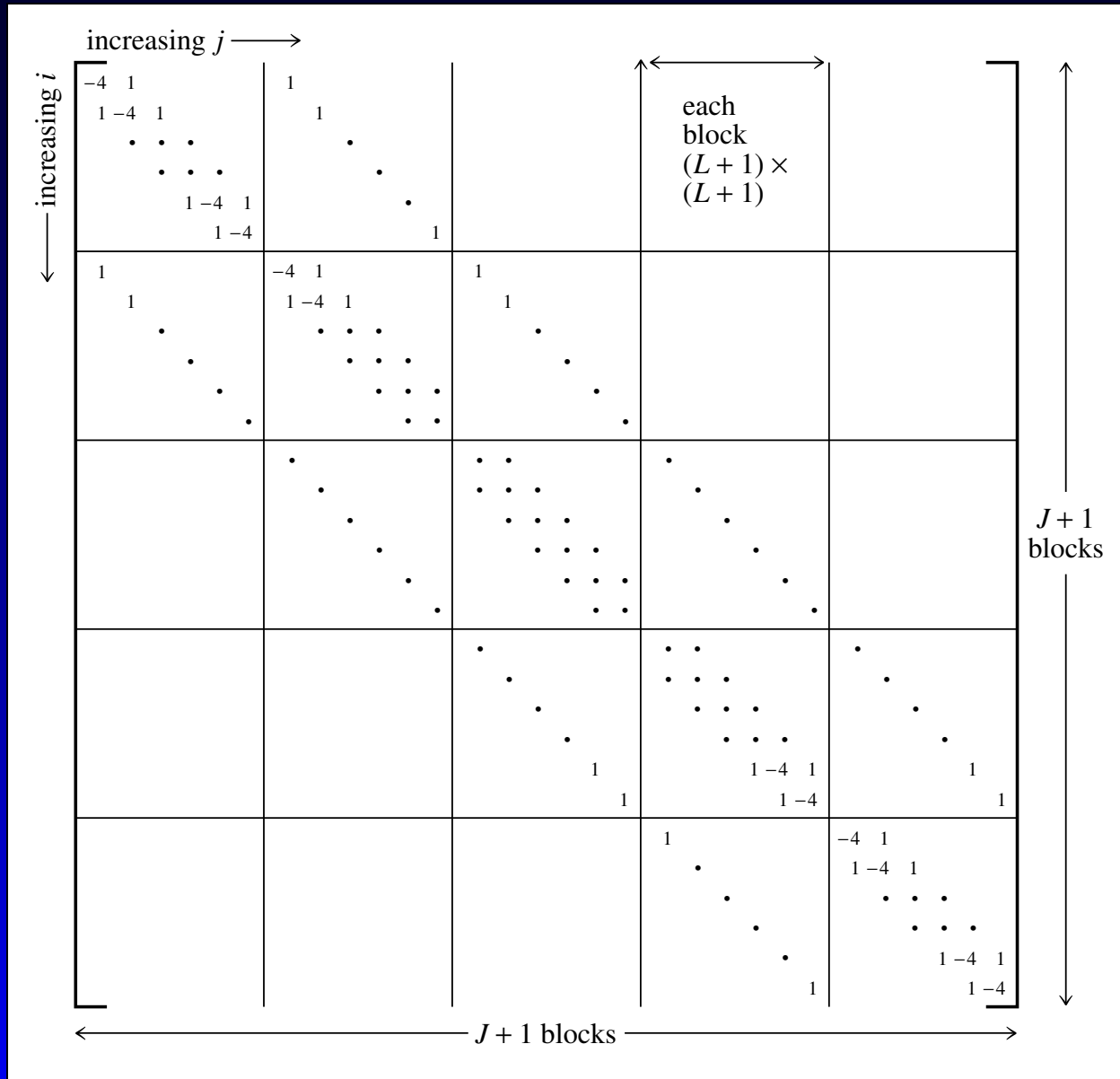
Finite Element Method

Features

- Flexibility

- Complicated geometries

- High-order approximations

- Strong mathematical foundation

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

1D Elliptic Example

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

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

- For example, elastic cord with fixed ends
- Solution must be twice differentiable
- This is unnecessarily strong if f is discontinuous

Weak Formulation

Multiply both sides by an arbitrary test function v and integrate

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

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

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

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

Weak Formulation 2

Find $u \in V$ such that

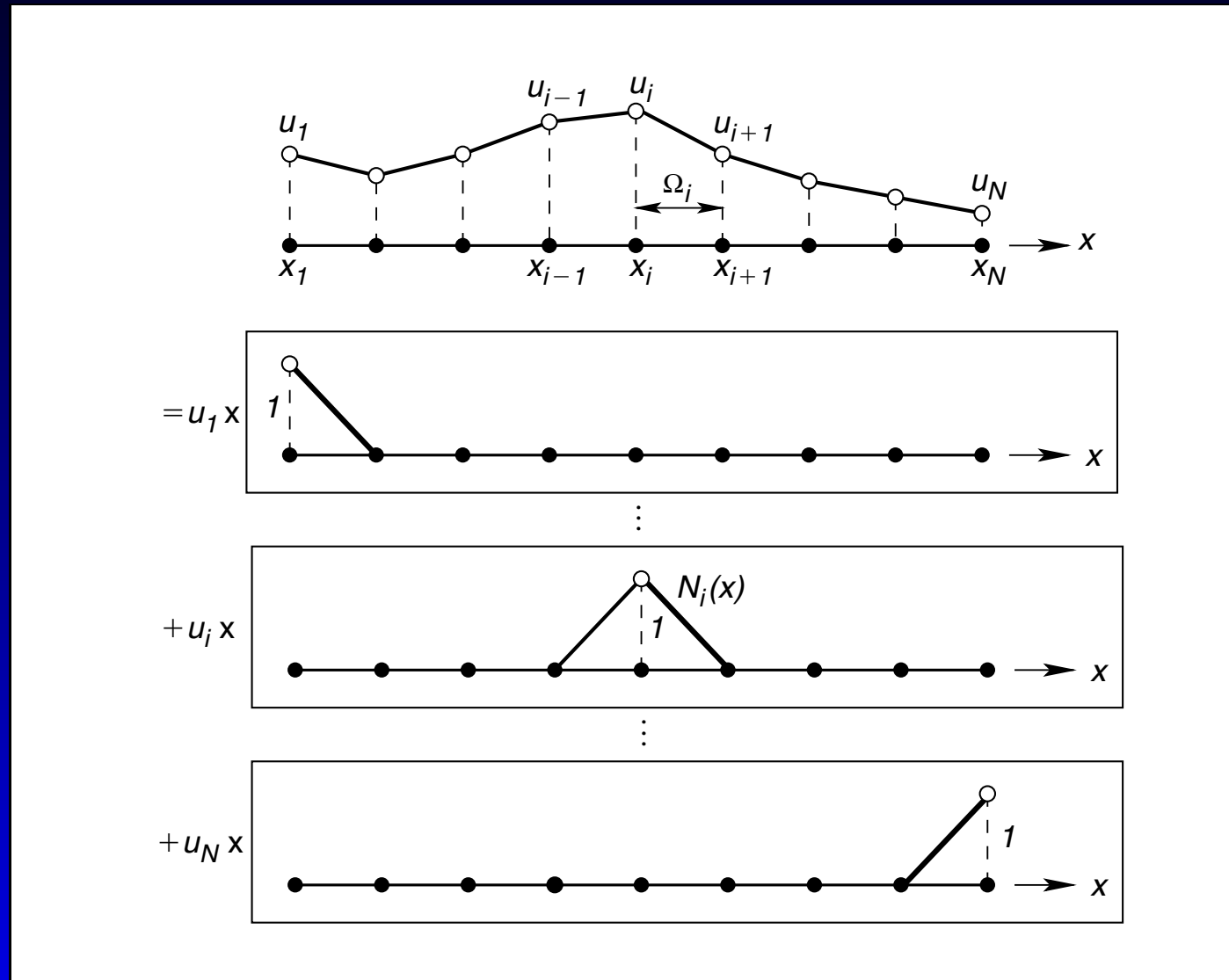$$\int_0^1 u'v'dx = \int_0^1 fvdx \qquad \forall v \in V$$

where $V = H_0^1([0,1])$.

- Fewer derivatives required for u
- If f continuous, same u as strong form
- Infinite possibilities for v
- Want to find u on a discrete mesh

Finite-dimensional Subspace

- Let $0 = x_0 < x_1 < \ldots < x_{M+1} = 1$ be a partition of the domain with $h_j = x_j - x_{j-1}$ and $h = \max h_j$. Use the partition to define a finite-dimensional subspace $V_h \subset V$.

- For decreasing h, want that functions in V_h can get arbitrarily close to functions in V.

- For example, let V_h be piecewise linear (i.e., on each subinterval) functions such that $\hat{v} \in V_h$ is continuous on $[0, 1]$ and $\hat{v}(0) = \hat{v}(1) = 0$.

- We may introduce *basis functions* $\phi_j(x)$ such that $\phi_j(x_i) = \delta_{ij}$ for $i, j = 0, \ldots, M + 1$.

- Nodes x_i are sometimes denoted N_i

Basis Functions

Finite Element Method

Find $\hat{u} \in V_h$ such that

$$\int_0^1 \hat{u}'\hat{v}'dx = \int_0^1 f\hat{v}dx \qquad \forall \hat{v} \in V_h.$$

or

$$\int_0^1 \hat{u}'\phi_j'dx = \int_0^1 f\phi_j dx \qquad j = 1, \ldots, M.$$

Note:

- When $\hat{u}$ and $\hat{v}$ in same subspace: Galerkin
- If support of ϕ_i is entire space: Spectral
- If V_h not a subspace of V: Non-conforming

Linear System

- Can represent $\hat{u} = \sum_{i=1}^{M} \xi_i \phi_i(x)$

- Find ξ_i for $i = 1, \ldots, M$ such that

$$\int_0^1 \sum_{i=1}^{M} \xi_i \phi_i' \phi_j' \, dx = \int_0^1 f \phi_j \, dx \qquad j = 1, \ldots, M.$$

- 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

$$A\xi = b$$

Stiffness Matrix

- The $M \times M$ matrix A is called the stiffness matrix.

- For the piecewise linear basis functions we have chosen it will be tridiagonal.

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

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

Compare to FDM

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

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

  which are exactly the same as FDM.

- The advantage of the FEM formulation is the generality it allows (e.g., uniform h was not required).

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Multidimensional Problem

- Let Ω be the unit square $(x, y) \in [0, 1] \times [0, 1]$

- Assume homogeneous Dirichlet boundary conditions

- Then the 2D Possion problem is:
  Find $u \in V := H_0^1(\Omega)$ such that

$$-\Delta u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial\Omega.$$

Variational Formulation

Find $u \in V$ such that

$$a(u,v)_\Omega = (f,v)_\Omega, \quad \forall v \in V,$$

where
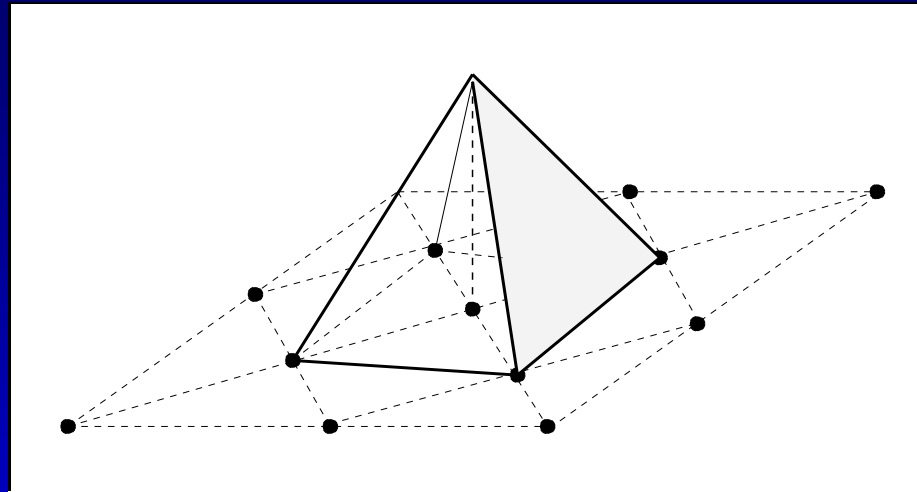
$$a(u,v)_\Omega := \int_\Omega \nabla u \cdot \nabla v,$$

$$(f,v)_\Omega := \int_\Omega fv.$$

Note: used Green's formula and $v = 0$ on $\partial\Omega$.

P_1 **Finite Element**

We introduce a triangulation T_h of Ω into triangles K_i, and a finite dimensional subspace:

$$V_h := \{\hat{v} \in H_0^1(\Omega) : \hat{v}|_{K_i} \in P_1(K_i)\}.$$

Find $\hat{u} \in V_h$ such that

$$a(\hat{u}, \hat{v})_\Omega = (f, \hat{v})_\Omega, \quad \forall \hat{v} \in V_h.$$

Using Basis Functions

Representing $\hat{u}$ and $\hat{v}$ in terms of nodal basis functions $\{\phi_i\}_{i=1}^M$ of V_h, i.e., $\phi_j(N_i) = \delta_{ij}$ for $i, j = 0, \dots, M+1$, we get the following system of algebraic equations:

$$\sum_{j=1}^M \xi_j a(\phi_i, \phi_j) = (f, \phi_i), \qquad i = 1, \dots, M,$$

or in matrix form,

$$A\xi = b,$$

where $\xi_j = \hat{u}(N_j)$, $A_{ij} = a(\phi_i, \phi_j)_\Omega$ is SPD, and $b_i = (f, \phi_i)_\Omega$.

Multidimensional Problem

- Let Ω be the unit cube $\{x, y, z\} \in [0, 1]$

- Assume homogeneous Dirichlet boundary conditions

- Then the 3D Possion problem is:
  Find $u \in V := H_0^1(\Omega)$ such that

$$-\Delta u = f \quad \text{in } \Omega,$$
$$u = 0 \quad \text{on } \partial\Omega.$$

Variational Formulation

Find $u \in V$ such that

$$a(u, v)_\Omega = (f, v)_\Omega, \quad \forall v \in V,$$

where

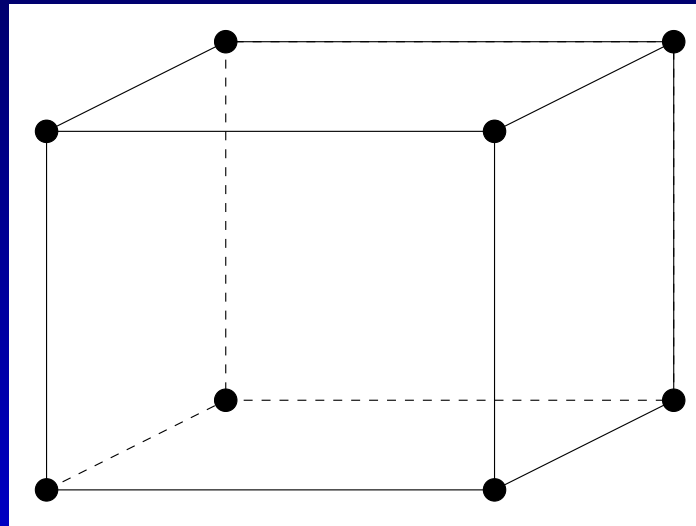$$a(u, v)_\Omega := \int_\Omega \nabla u \cdot \nabla v,$$

$$(f, v)_\Omega := \int_\Omega fv.$$

Note: used Green's formula and $v = 0$ on $\partial\Omega$.

Q_1 Finite Element

We introduce a triangulation T_h of Ω into 3-D rectangles K_i, and a finite dimensional subspace:

$$V_h := \{\hat{v} \in H_0^1(\Omega) : \hat{v}|_{K_i} \in Q_1(K_i)\}.$$

Find $\hat{u} \in V_h$ such that

$$a(\hat{u}, \hat{v})_\Omega = (f, \hat{v})_\Omega, \quad \forall \hat{v} \in V_h.$$

Using Basis Functions

Representing $\hat{u}$ and $\hat{v}$ in terms of nodal basis functions $\{\phi_i\}_{i=1}^{M}$ of V_h, i.e., $\phi_j(N_i) = \delta_{ij}$ for $i, j = 0, \ldots, M + 1$, we get the following system of algebraic equations:

$$\sum_{j=1}^{M} \xi_j a(\phi_i, \phi_j) = (f, \phi_i), \qquad i = 1, \ldots, M,$$

or in matrix form,

$$A\xi = b,$$

where $\xi_j = \hat{u}(N_j)$, $A_{ij} = a(\phi_i, \phi_j)_\Omega$ is SPD, and $b_i = (f, \phi_i)_\Omega$.

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Neumann Problem

- Let Ω be the unit square $(x, y) \in [0, 1] \times [0, 1]$

- Assume Neumann boundary conditions

- Then the 2D Possion problem is:
  Find $u \in V := H^1(\Omega)$ such that

$$-\Delta u = f \quad \text{in } \Omega,$$

$$\frac{\partial u}{\partial n} = g \quad \text{on } \partial\Omega.$$

Variational Formulation

Find $u \in V$ such that

$$a(u, v)_\Omega = (f, v)_\Omega + \langle g, v \rangle_{\partial\Omega}, \quad \forall v \in V,$$

where

$$a(u, v)_\Omega := \int_\Omega \nabla u \cdot \nabla v,$$
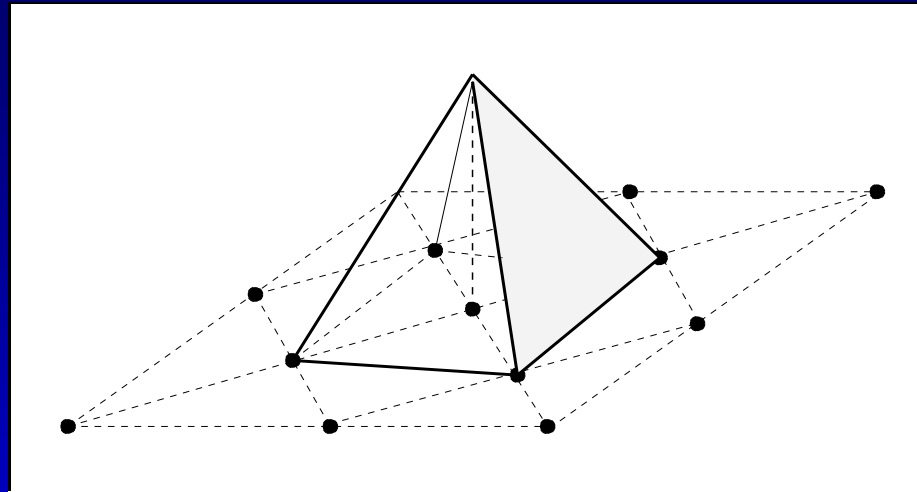
$$(f, v)_\Omega := \int_\Omega fv,$$

$$\langle g, v \rangle_{\partial\Omega} := \int_{\partial\Omega} gv.$$

Note: used Green's formula and $\frac{\partial u}{\partial n} = g$ on $\partial\Omega$.

P_1 **Finite Element**

We introduce a triangulation T_h of Ω into triangles K_i, and a finite dimensional subspace:

$$V_h := \{\hat{v} \in H^1(\Omega) : \hat{v}|_{K_i} \in P_1(K_i)\}.$$

Find $\hat{u} \in V_h$ such that

$$a(\hat{u}, \hat{v})_\Omega = (f, \hat{v})_\Omega + \langle g, \hat{v} \rangle_{\partial\Omega}, \quad \forall \hat{v} \in V_h.$$

Using Basis Functions

Representing $\hat{u}$ and $\hat{v}$ in terms of nodal basis functions $\{\phi_i\}_{i=0}^{M+1}$ of V_h, we get the following system of algebraic equations:

$$\sum_{j=0}^{M+1} \xi_j a(\phi_i, \phi_j) = (f, \phi_i) + \langle g, \phi_i \rangle_{\partial\Omega}, \quad i = 0, \ldots, M+1,$$
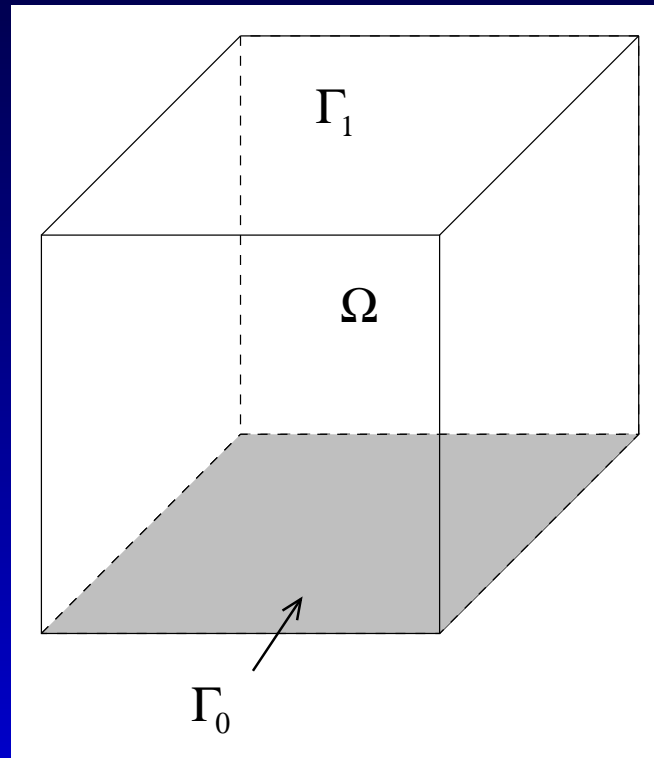
or in matrix form,

$$A\xi = b,$$

where $\xi_j = \hat{u}(N_j)$, $A_{ij} = a(\phi_i, \phi_j)_\Omega$ is SPD, and $b_i = (f, \phi_i)_\Omega + \langle g, \phi_i \rangle_{\partial\Omega}$.

Mixed Boundary

Let Ω be the unit cube, Γ_0 the face at $z = 0$, and $\Gamma_1 = \partial\Omega \setminus \Gamma_0$. Then we want to approximate u in Ω.

Mixed Robin Boundary

Find $u \in V := H^1(\Omega)$ such that

$$-\Delta u = f \qquad \text{in } \Omega,$$

$$\alpha_0 u + \beta_0 \frac{\partial u}{\partial n} = 0 \qquad \text{on } \Gamma_0,$$

$$\alpha_1 u + \beta_1 \frac{\partial u}{\partial n} = 0 \qquad \text{on } \Gamma_1.$$

Note: assume $\beta_i \neq 0$.

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Variational Formulation

Find $u \in V$ such that

$$a(u, v)_\Omega - \left\langle \frac{\partial u}{\partial n}, v \right\rangle_{\Gamma_0} - \left\langle \frac{\partial u}{\partial n}, v \right\rangle_{\Gamma_1} = (f, v)_\Omega,$$

or

$$a(u, v)_\Omega + \alpha_0 \beta_0^{-1} \langle u, v \rangle_{\Gamma_0} + \alpha_1 \beta_1^{-1} \langle u, v \rangle_{\Gamma_1} = (f, v)_\Omega,$$

where $a(u, v)_\Omega$ and $(f, v)_\Omega$ are the same as above and

$$\langle u, v \rangle_{\Gamma_j} := \int_{\Gamma_j} uv, \quad j = 0, 1.$$

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Finite Element Method

We introduce the triangulation T_h as before, and the finite dimensional subspace

$$V_h := \{\hat{u} \in H^1(\Omega) : \hat{u}|_{K_i} \in Q_1(K_i)\}$$

to get the finite element problem:
Find $\hat{u} \in V_h$ such that

$$a(\hat{u}, \hat{v})_\Omega + \alpha_0 \beta_0^{-1} \langle \hat{u}, \hat{v} \rangle_{\Gamma_0} + \alpha_1 \beta_1^{-1} \langle \hat{u}, \hat{v} \rangle_{\Gamma_1}$$
$$= (f, \hat{v})_\Omega, \quad \forall \hat{v} \in V_h.$$

Using Basis Functions

Representing $\hat{u}$ and $\hat{v}$ in terms of nodal basis functions $\{\phi_i\}_{i=1}^M$ of V_h we get the following matrix equation:

$$(A + G)\xi = b,$$

where ξ, A, and b are similar to those above and

$$G_{ij}^0 := \langle \phi_i, \phi_j \rangle_{\Gamma_0},$$

$$G_{ij}^1 := \langle \phi_i, \phi_j \rangle_{\Gamma_1},$$

$$G := \frac{\alpha_0}{\beta_0} G^0 + \frac{\alpha_1}{\beta_1} G^1.$$

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Parabolic and Elliptic

- Build off of elliptic FEM

- If boundary not moving, space-time rectangular in t dimension

- Popular to use FEM for spatial discretization and FDM for time

- Performing FEM first results in semi-discrete formulation

- This is equivalent to a coupled system of ODEs

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Scalar Wave Problem

Find $u \in H^2([0, T]; L^2(\Omega)) \cap L^2([0, T]; H_0^1(\Omega))$ such that

$$\frac{1}{c^2} u_{tt} - \Delta u = f \qquad \text{in } \Omega,$$

$$u = 0 \qquad \text{in } \partial\Omega \times (0, T),$$

$$u(\cdot, 0) = u_0(\cdot) \qquad \text{in } \Omega,$$

$$u_t(\cdot, 0) = u_1(\cdot) \qquad \text{in } \Omega.$$

Variational Formulation

Find $u(\cdot, t) : [0, T] \rightarrow V := H_0^1(\Omega)$ such that

$$\frac{1}{c^2}(u_{tt}, v)_\Omega + a(u, v)_\Omega = (f, v)_\Omega, \qquad \forall v \in V,$$

$$(u(\cdot, 0), v)_\Omega = (u_0(\cdot), v)_\Omega, \qquad \forall v \in V,$$

$$(u_t(\cdot, 0), v)_\Omega = (u_1(\cdot), v)_\Omega, \qquad \forall v \in V.$$

Semi-discrete Formulation

Find $\hat{u}(\cdot, t) : [0, T] \to V_h$ such that

$$\frac{1}{c^2}(\ddot{u}_h, \hat{v})_\Omega + a(\hat{u}, \hat{v})_\Omega = (f, \hat{v})_\Omega, \qquad \forall \hat{v} \in V_h,$$

$$(\hat{u}(\cdot, 0), \hat{v})_\Omega = (u_0(\cdot), \hat{v})_\Omega, \qquad \forall \hat{v} \in V_h,$$

$$(\dot{u}_h(\cdot, 0), \hat{v})_\Omega = (u_1(\cdot), \hat{v})_\Omega, \qquad \forall \hat{v} \in V_h.$$

Using Basis Functions

In matrix form,

$$\frac{1}{c^2}L\ddot{\xi}(t) + A\xi(t) = b, \qquad \forall t \in (0, T),$$

$$L\xi(0) = \chi^0,$$

$$L\dot{\xi}(0) = \chi^1,$$

where ξ, A, and b are as above, and

$$\chi_i^0 := (u_0, \phi_i)_\Omega,$$

$$\chi_i^1 := (u_1, \phi_i)_\Omega,$$

$$L_{ij} := (\phi_i, \phi_j)_\Omega.$$

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Fully Discrete Formulation

In order to discretize in time, we introduce a (uniform) partition of the interval [0,T]:
$0 = t_0 < t_1 < \cdots < t_{N_T} = T$, and
$k := t_n - t_{n-1}, n = 1, \ldots, N_T$.

$$\frac{1}{c^2} L \frac{\xi^{n+1} - 2\xi^n + \xi^{n-1}}{k^2} + A\xi^n = b^n, \quad n = 1, \ldots, N_T,$$

$$L\xi^0 = \chi^0,$$

$$L\xi^1 = \chi^0 + k\chi^1,$$

where $\xi_i^n \approx \xi_i(t_n)$ and $b_i^n := b_i(t_n)$.

Mass Lumping

- Note that the fully discrete formulation is still implicit, thus a linear solve at each time step must be performed.

- Since $L_{ij} := (\phi_i, \phi_j)_\Omega$, it is possible to make L diagonal by using a quadrature rule (Trapezoid) for the integration.

- The resulting explicit method is exactly the FDM.

- When to lump is an important question; numerical dispersion analysis can show, for example, in 1D consistent mass matrix requires a smaller time step than lumped, and a linear solve!

- Mass lumping can reduce accuracy, especially in higher dimensions.

Other Considerations

- Integration performed in "local" coordinates, then global matrix assembled.

- K may be mapped to reference domain (e.g., $[-1, 1]$) for easy integration (especially quadrature rules).

- Technically speaking a finite element is a triple: geometric object, finite-dimensional linear function space, and a set of degrees of freedom.

- Many types of finite elements exist, including some with quadratic or cubic basis functions, first or second derivatives as degrees of freedom, or degrees of freedom in locations other than vertices (e.g., centroid).

- More general than FDM, and more easily applied to slanted or curved boundaries, especially involving normal derivative boundary conditions.

Conservation Laws

- Many PDEs are derived from physical models called *conservation laws*.

- The general principle is that the rate of change of $u(\mathbf{x}, t)$ within a volume V is equal to the flux past the boundary

$$\frac{\partial}{\partial t} \int_V u(\mathbf{x}, t) + \int_{\partial V} \mathbf{f}(u) \cdot \mathbf{n} = 0$$

where $\mathbf{f}$ is flux function.

- Nonlinear conservation laws can result in discontinuities in finite time even with smooth initial data.

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Finite Volume Method

- Rather than pointwise approximations on a grid, FVM approximates the average integral value on a reference volume.

- Suppose region $V_i = \left[x_{i-(1/2)}, x_{i+(1/2)} \right]$ then

$$\int_{x_{i-(1/2)}}^{x_{i+(1/2)}} u_t dx + f(u_{i+(1/2)}) - f(u_{i-(1/2)}) = 0$$

  where we have applied Gauss's theorem and integrated analytically the resulting term $\int_{x_{i-(1/2)}}^{x_{i+(1/2)}} f_x(u) dx$.

- We can apply a quadrature rule, for example Midpoint, to the remaining integral to get a semi-discrete form

$$\left(x_{i+(1/2)} - x_{i-(1/2)} \right) u_t(x_i) + f(u_{i+(1/2)}) - f(u_{i-(1/2)}) = 0.$$

FVM Example

Consider the elliptic equation $u_{xx} = f(x)$ on a control volume $V_i = \left[x_{i-(1/2)}, x_{i+(1/2)} \right]$ then

$$\int_{x_{i-(1/2)}}^{x_{i+(1/2)}} u_{xx} dx = \int_{x_{i-(1/2)}}^{x_{i+(1/2)}} f dx.$$

Evaluating the left hand side analytically and the right via Midpoint gives

$$u_x(x_{i+(1/2)}) - u_x(x_{i-(1/2)}) = \left(x_{i+(1/2)} - x_{i-(1/2)} \right) f_i$$

Finally, using centered differences on the remaining derivatives yields

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

for $h = x_{i+(1/2)} - x_{i-(1/2)}$.

FVM Summary

- Applies to integral form of conservation law.

- Handles discontinuities in solutions.

- Natural choice for heterogeneous material as each grid cell can be assigned different material parameters.

- There exist theory for convergence, accuracy and stability.

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Systems of Linear Equations

- For implicit methods must choose a linear solver.

- Direct (LU factorization)
  - More accurate
  - May be cheaper for many time steps
  - Banded (otherwise fill-in)

- Iterative
  - If accuracy less important than speed
  - Matrix-free
  - Sparse
  - SPD

Iterative Methods

- Successive Over Relaxation (SOR)
  - Simple to code
  - $\omega = 1$ is Gauss-Seidel
- Conjugate Gradient
  - SPD
  - Eigenvalues clustered together (Precondition)
- Generalized Minimum Residual (GMRES)
  - Non-SPD, e.g. convection-diffusion with upwinding
  - Krylov method: builds orthonormal basis which may get big (Restart)
  - Preconditioning helps (Incomplete Cholesky)