SOLUTION OF

Partial Differential Equations

(PDEs)

Mathematics is the Language of Science

PDEs are the expression of processes that occur across time & space: (x,t), (x,y), (x,y,z), or (x,y,z,t)

Partial Differential Equations (PDE's)

A **PDE** is an equation which includes derivatives of an unknown function with respect to **2 or more** independent variables

Partial Differential Equations (PDE's)

PDE's describe the behavior of many engineering phenomena:

- Wave propagation
- Fluid flow (air or liquid)
  - Air around wings, helicopter blade, atmosphere
  - Water in pipes or porous media
  - Material transport and diffusion in air or water
  - Weather: large system of coupled PDE's for momentum, pressure, moisture, heat, …
- Vibration
- Mechanics of solids:
  - stress-strain in material, machine part, structure
- Heat flow and distribution
- Electric fields and potentials
- Diffusion of chemicals in air or water
- Electromagnetism and quantum mechanics

Partial Differential Equations (PDE's)

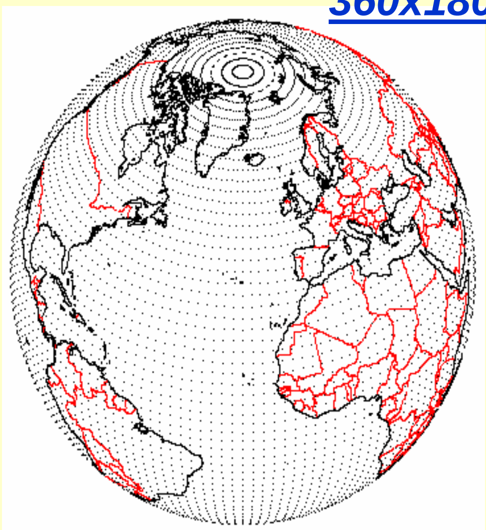
Weather Prediction

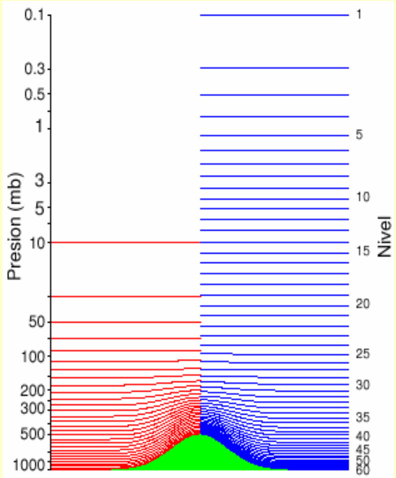
- heat transport & cooling
- advection & dispersion of moisture
- radiation & solar heating
- evaporation
- air (movement, friction, momentum, coriolis forces)
- heat transfer at the surface

To predict weather one need "only" solve a very large systems of coupled PDE equations for momentum, pressure, moisture, heat, etc.

Modelización Numérica del Tiempo

360x180x32 x nvar





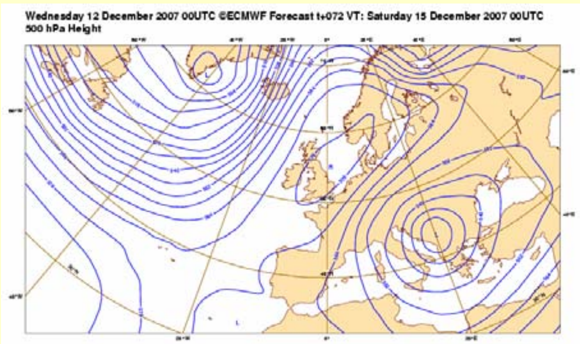
Conservación de energía, masa, momento, vapor de agua, ecuación de estado de gases.

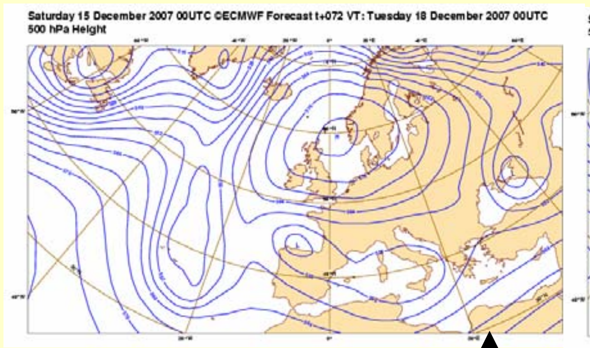
$$
\left\{
\begin{aligned}
\frac{d\boldsymbol{v}}{dt} &= -\alpha\boldsymbol{\nabla}p - \boldsymbol{\nabla}\phi + \boldsymbol{F} - 2\boldsymbol{\Omega}\times\boldsymbol{v} \\
\frac{\partial\rho}{\partial t} &= -\boldsymbol{\nabla}\cdot(\rho\,\boldsymbol{v}) \\
p\,\alpha &= RT \\
Q &= C_p\frac{dT}{dt} - \alpha\frac{dp}{dt} \\
\frac{\partial\rho\,q}{\partial t} &= -\boldsymbol{\nabla}\cdot(\rho\,\boldsymbol{v}\,q) + \rho\,(E-C)
\end{aligned}
\right.
$$

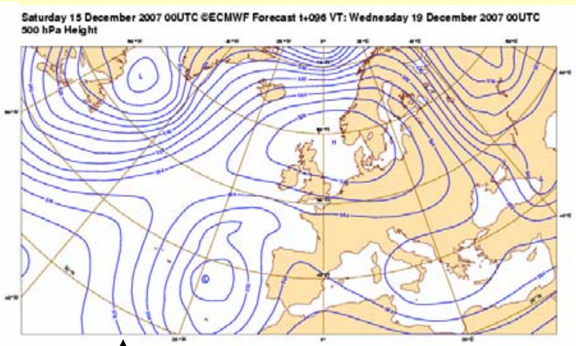
$\boldsymbol{v}$ = (u, v, w), T, p, $\rho = 1/\alpha$ y q

resolución $\propto$ 1/Δt

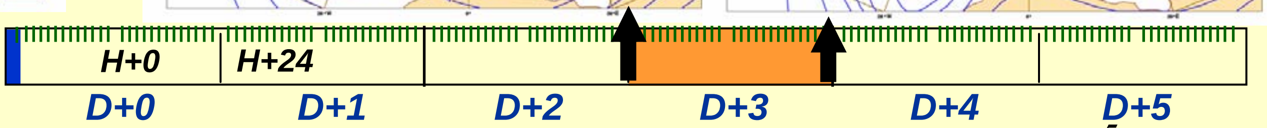
*Duplicar la resolución espacial supone incrementar el tiempo de cómputo en un factor **16***







Condición inicial



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Partial Differential Equations (PDE's)

Learning Objectives

1) Be able to distinguish between the 3 classes of 2nd order, linear PDE's. Know the physical problems each class represents and the physical/mathematical characteristics of each.

2) Be able to describe the differences between finite-difference and finite-element methods for solving PDEs.

3) Be able to solve Elliptical (Laplace/Poisson) PDEs using finite differences.

4) Be able to solve Parabolic (Heat/Diffusion) PDEs using finite differences.

Partial Differential Equations (PDE's)

Engrd 241 Focus:

Linear 2nd-Order PDE's of the general form

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D = 0$$

u(x,y), A(x,y), B(x,y), C(x,y), and D(x,y,u,,)

The PDE is nonlinear if A, B or C include u, $\partial u/\partial x$ or $\partial u/\partial y$, or if D is nonlinear in u and/or its first derivatives.

Classification

$B^2 - 4AC < 0$	——> Elliptic	(e.g. Laplace Eq.)
$B^2 - 4AC = 0$	——> Parabolic	(e.g. Heat Eq.)
$B^2 - 4AC > 0$	——> Hyperbolic	(e.g. Wave Eq.)

- Each category describes different phenomena.
- Mathematical properties correspond to those phenomena.

Partial Differential Equations (PDE's)

Elliptic Equations ($B^2 - 4AC < 0$) [steady-state in time]

- typically characterize steady-state systems (no time derivative)
  - temperature
  - pressure
  - electrical potential
  - torsion
  - membrane displacement
- closed domain with boundary conditions expressed in terms of

$$u(x, y), \qquad \frac{\partial u}{\partial \eta} \text{ (in terms of } \frac{\partial u}{\partial x} \text{ and } \frac{\partial u}{\partial y}\text{)}$$

Typical examples include

$$\nabla^2 u \equiv \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \begin{cases} 0 & \textbf{Laplace Eq.} \\ -D(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) & \textbf{Poisson Eq.} \end{cases}$$

$$A = 1,\ B = 0,\ C = 1 \quad ==> \quad B^2 - 4AC = -4 < 0$$

Elliptic PDEs

Boundary Conditions for Elliptic PDE's:

Dirichlet: u provided along all of edge

Neumann: $\frac{\partial u}{\partial \eta}$ provided along all of the edge (derivative in normal direction)

Mixed: u provided for some of the edge and

$\frac{\partial u}{\partial \eta}$ for the remainder of the edge

Elliptic PDE's are analogous to Boundary Value ODE's

Elliptic PDEs

u(x,y =1) or ∂u/∂y given on boundary

y

u(x=0,y)
or
∂u/∂x
given
on
boundary

Estimate
u(x)
from
Laplace
Equations

u(x=1,y)
or
∂u/∂x
given
on
boundary

u(x,y =0) or ∂u/∂v given on boundary

x

Parabolic PDEs

Parabolic Equations (B^2 – 4AC = 0) [first derivative in time]

- variation in both space (x,y) and time, t
- typically provided are:
  - initial values: $u(x,y,t = 0)$
  - boundary conditions: $u(x = x_o, y = y_o, t)$ for all t

    $u(x = x_f, y = y_f, t)$ for all t

- all changes are propagated forward in time, i.e., nothing goes backward in time; changes are propagated across space at decreasing amplitude.

Parabolic PDEs

Parabolic Equations ($B^2 - 4AC = 0$) [first derivative in time]

- Typical example: **Heat Conduction or Diffusion**

(the Advection-Diffusion Equation)

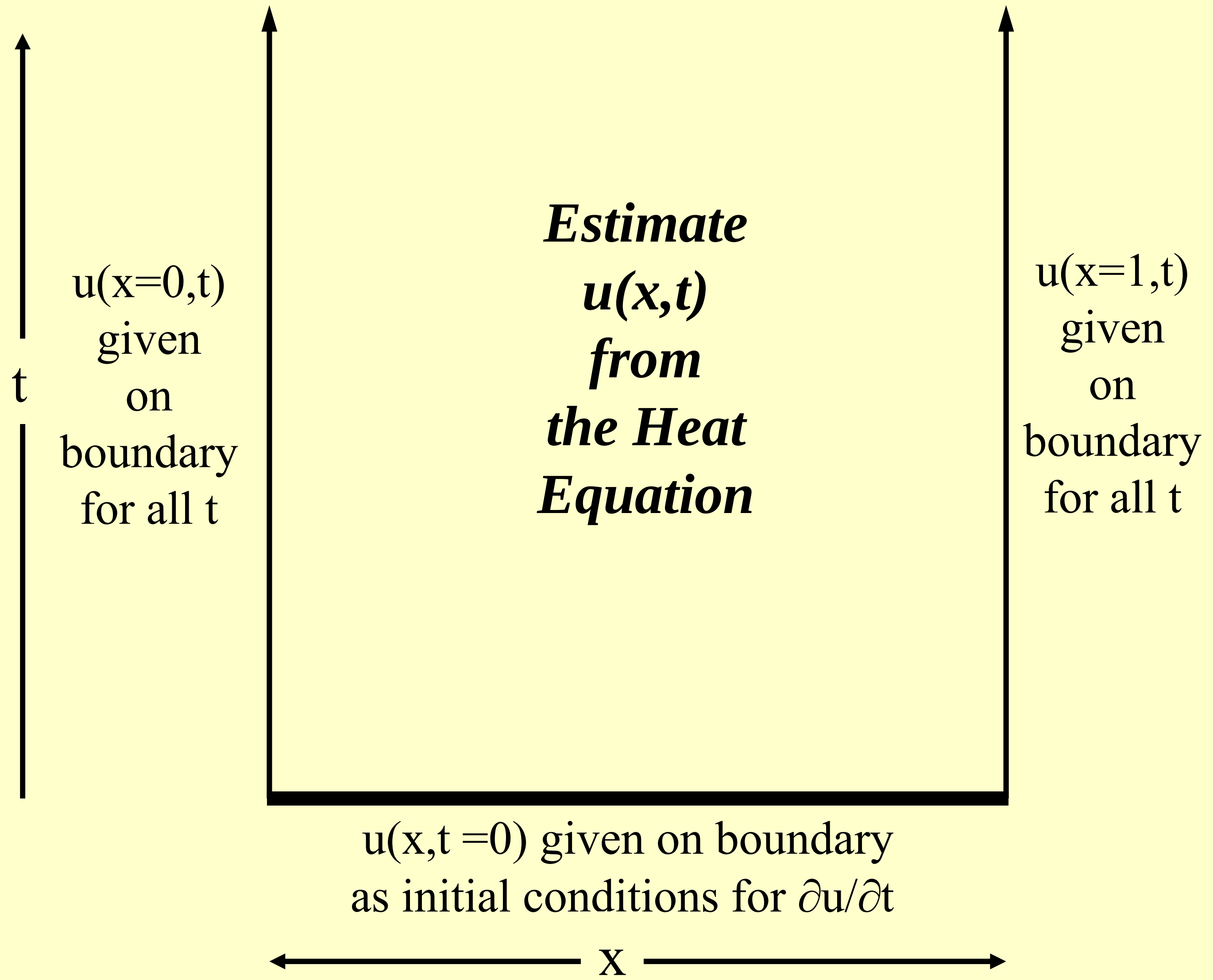
$$\text{1D}: \quad \frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2} + \bar{D}(x, u, \frac{\partial u}{\partial x})$$

$$A = k,\ B = 0,\ C = 0 \text{ –> } B^2 - 4AC = 0$$

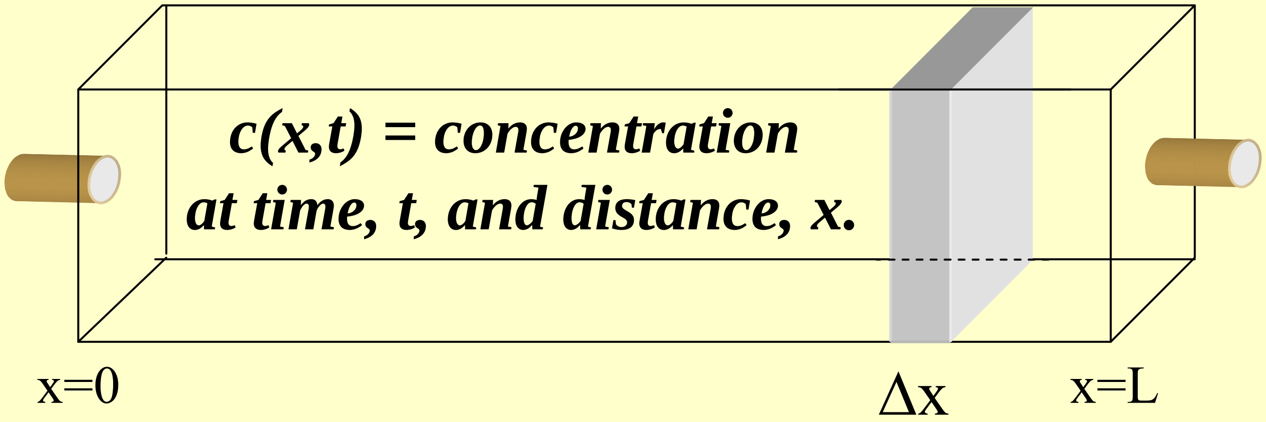
$$\text{2D}: \quad \frac{\partial u}{\partial t} = k\left[\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right] + \bar{D}(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y})$$

$$= k\ \nabla^2 u + \bar{D}$$

Parabolic PDEs

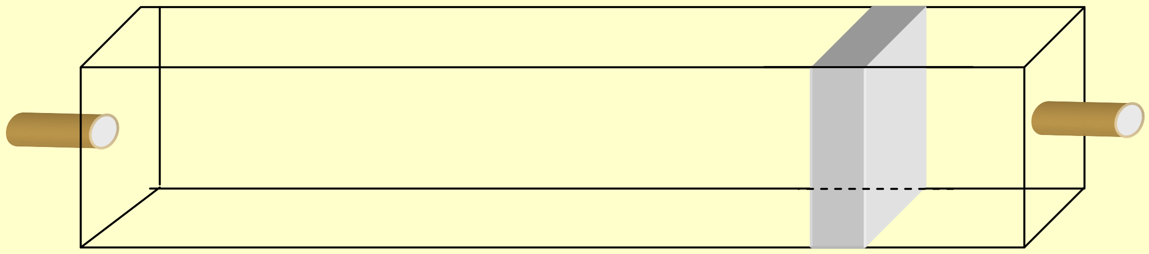


Parabolic PDEs



- An elongated reactor with a single entry and exit point and a uniform cross-section of area A.
- A mass balance is developed for a finite segment Δx along the tank's longitudinal axis in order to derive a differential equation for concentration ($V = A\,\Delta x$).

Parabolic PDEs



$$V\frac{\Delta c}{\Delta t} = Q\,c(x) - Q\left[c(x) + \frac{\partial c(x)}{\partial x}\Delta x\right] - D\,A\frac{\partial c(x)}{\partial x}$$

Flow in **Flow out** **Dispersion in**

$$+\,D\,A\left[\frac{\partial c(x)}{\partial x} + \frac{\partial}{\partial x}\frac{\partial c(x)}{\partial x}\Delta x\right] - k\,V\,c(x)$$

Dispersion out **Decay reaction**

As Δt and Δx ==> 0 $\qquad \dfrac{\Delta c}{\Delta t} \Longrightarrow \dfrac{\partial c}{\partial t} = D\dfrac{\partial^2 c}{\partial x^2} - \dfrac{Q}{A}\dfrac{\partial c}{\partial x} - kc$

Hyperbolic PDEs

Hyperbolic Equations ($B^2 - 4AC > 0$) [2nd derivative in time]

- variation in both space (x, y) and time, t
- requires:
  - initial values: $u(x,y,t=0)$, $\partial u/\partial t\ (x,y,t = 0)$ "initial velocity"
  - boundary conditions: $u(x = x_o, y = y_o, t)$ for all t
    $u(x = x_f, y = y_f, t)$ for all t
- all changes are propagated forward in time, i.e., nothing goes backward in time.

Hyperbolic PDEs

Hyperbolic Equations (B^2 – 4AC > 0) [2nd derivative in time]

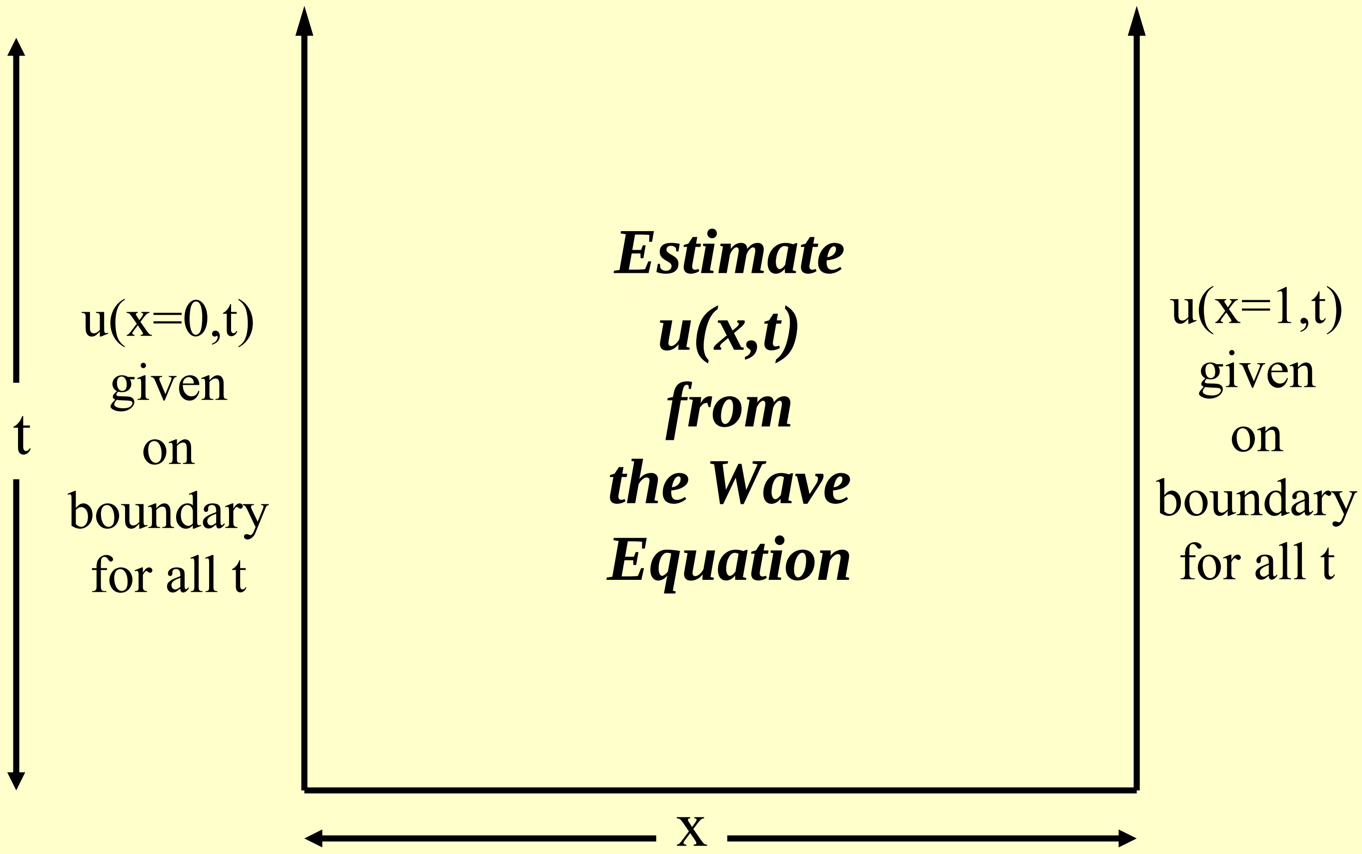
- Typical example: **Wave Equation**

$$1D: \quad \frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} + D(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial t}) = 0$$

$A = 1, \; B = 0, \; C = -1/c^2 \implies B^2 - 4AC = 4/c^2 > 0$

- Models
  - vibrating string
  - water waves
  - voltage change in a wire

Hyperbolic PDEs



$u(x,t=0)$ <u>and</u> $\partial u(x,t=0)/\partial t$
given on boundary
as initial conditions for $\partial^2 u/\partial t^2$

Now PDE is second order in time

Numerical Methods for Solving PDEs

Numerical methods for solving different types of PDE's reflect the different character of the problems.

- ***Laplace*** - solve all at once for steady state conditions
- ***Parabolic*** (heat) and ***Hyperbolic*** (wave) equations.
  Integrate initial conditions forward through time.

Methods

- **Finite Difference (FD) Approaches (C&C Chs. 29 & 30)**
  Based on approximating solution at a finite # of points, usually arranged in a regular grid.
- **Finite Element (FE) Method (C&C Ch. 31)**
  Based on approximating solution on an assemblage of simply shaped (triangular, quadrilateral) finite pieces or "elements" which together make up (perhaps complexly shaped) domain.

In this course, we concentrate on FD applied to elliptic and parabolic equations.

Finite Difference for Solving Elliptic PDE's

Solving Elliptic PDE's:

- Solve all at once
- Liebmann Method:
  - Based on Boundary Conditions (BCs) and finite difference approximation to formulate system of equations
  - Use Gauss-Seidel to solve the system

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \begin{cases} 0 & \textbf{Laplace Eq.} \\ -D(x, y, u, \dfrac{\partial u}{\partial x}, \dfrac{\partial u}{\partial y}) & \textbf{Poisson Eq.} \end{cases}$$

Finite Difference Methods for Solving Elliptic PDE's

1. Discretize domain into grid of evenly spaced points
2. For nodes where u is unknown:

$$\frac{\partial^2 u}{\partial x^2} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{(\Delta x)^2} + O(\Delta x^2)$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{(\Delta y)^2} + O(\Delta y^2)$$

w/ $\Delta x = \Delta y = h$, substitute into main equation

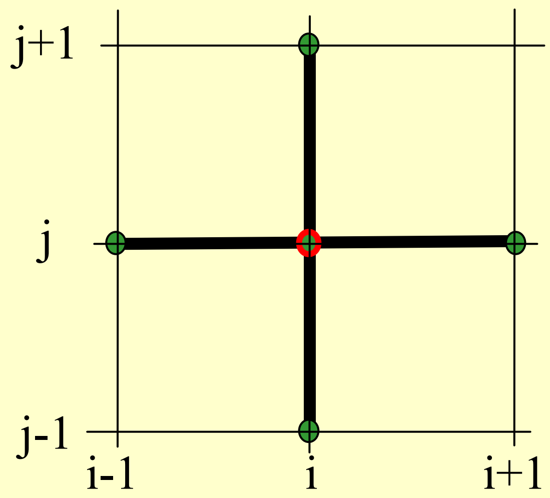
$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}}{h^2} + O(h^2)$$

3. Using Boundary Conditions, write, n*m equations for $u(x_{i=1:m}, y_{j=1:n})$ or n*m unknowns.
4. Solve this banded system with an efficient scheme. Using Gauss-Seidel iteratively yields the *Liebmann Method*.

Elliptical PDEs

The Laplace Equation $$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0$$

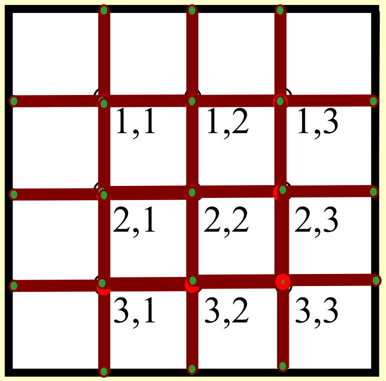
The Laplace molecule



If $\Delta x = \Delta y$ then $$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$$

Elliptical PDEs

The Laplace molecule: $T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$



The temperature distribution can be estimated by discretizing the Laplace equation at 9 points and solving the system of linear equations.

$$
\begin{array}{c}
\begin{array}{ccccccccc} T_{11} & T_{12} & T_{13} & T_{21} & T_{22} & T_{23} & T_{31} & T_{32} & T_{33} \end{array} \\
\begin{bmatrix}
-4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4
\end{bmatrix}
\end{array}
\begin{Bmatrix} T_{11} \\ T_{12} \\ T_{13} \\ T_{21} \\ T_{22} \\ T_{23} \\ T_{31} \\ T_{32} \\ T_{33} \end{Bmatrix}
=
\begin{Bmatrix} -100 \\ -100 \\ -200 \\ 0 \\ 0 \\ -100 \\ 0 \\ 0 \\ -100 \end{Bmatrix}
$$

Excel

Solution of Elliptic PDE's: Additional Factors

- Primary (solve for first):

  $u(x,y) = T(x,y)$ = temperature distribution

- Secondary (solve for second):

  heat flux: $q_x = -k' \dfrac{\partial T}{\partial x}$ and $q_y = -k' \dfrac{\partial T}{\partial y}$

  obtain by employing:

$$\frac{\partial T}{\partial x} \approx \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x} \qquad \frac{\partial T}{\partial y} \approx \frac{T_{i,j+1} - T_{i,j-1}}{2\Delta y}$$

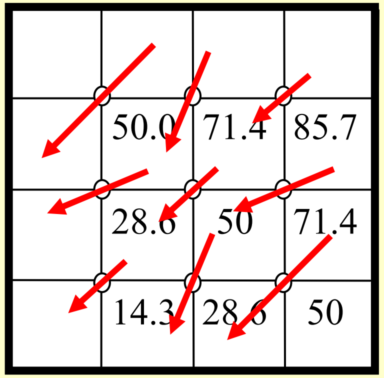
  then obtain resultant flux and direction:

$$q_n = \sqrt{q_x^2 + q_y^2} \qquad \theta = \tan^{-1}\left(\frac{q_y}{q_x}\right) \quad q_x > 0$$

$$\theta = \tan^{-1}\left(\frac{q_y}{q_x}\right) + \pi \quad q_x < 0$$

(with θ in radians)

Elliptical PDEs: additional factors



$$q_x = -k' \frac{\partial T}{\partial x} \approx -k' \frac{T_{i+1,j} - T_{i-1,j}}{2\Delta x}$$

$$q_y = -k' \frac{\partial T}{\partial y} \approx -k' \frac{T_{i,j+1} - T_{i,j-1}}{2\Delta y}$$

$k' = 0.49$ cal/s·cm·°C

At point 2,1 (middle left):

$q_x \sim -0.49\ (50-0)/(2\cdot 10\text{cm}) = -1.225\ \text{cal}/(\text{cm}^2\cdot\text{s})$

$q_y \sim -0.49\ (50-14.3)/(2\cdot 10\text{cm}) = -0.875\text{cal}/(\text{cm}^2\cdot\text{s})$

$$q_n = \sqrt{q_x{}^2 + q_y{}^2} = \sqrt{1.225^2 + 0.875^2} = 1.851\,\text{cal}/(\text{cm}^2\cdot\text{s})$$

$$\theta = \tan^{-1}\left(\frac{q_y}{q_x}\right) = \tan^{-1}\left(\frac{-0.875}{-1.225}\right) = 35.5^o + 180^o = 215.5^o$$

Solution of Elliptic PDE's: Additional Factors

Neumann Boundary Conditions (derivatives at edges)

- employ phantom points outside of domain
- use FD to obtain information at phantom point,

$$T_{1,j} + T_{-1,j} + T_{0,j+1} + T_{0,j-1} - 4T_{0,j} = 0 \quad [*]$$

If given $\frac{\partial T}{\partial x}$ then use $\frac{\partial T}{\partial x} = \frac{T_{1,j} - T_{i-1,j}}{2\Delta x}$

to obtain $T_{-1,j} = T_{1,j} - 2\Delta x \frac{\partial T}{\partial x}$

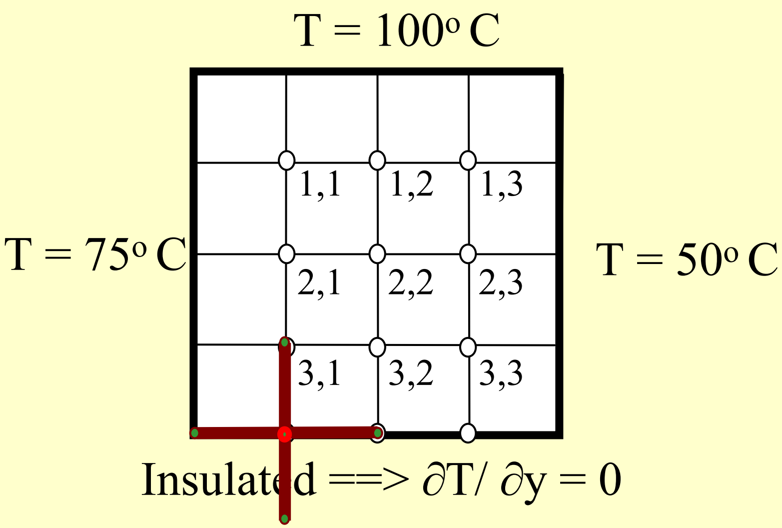
Substituting [*]: $2T_{1,j} - 2\Delta x \frac{\partial T}{\partial x} + T_{0,j+1} + T_{0,j-1} - 4T_{0,j} = 0$

Irregular boundaries

- use unevenly spaced molecules close to edge
- use finer mesh

Elliptical PDEs: Derivative Boundary Conditions

The Laplace molecule: $T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4T_{i,j} = 0$



Derivative (Neumann) BC at (4,1):

$$\frac{\partial T}{\partial y} = \frac{T_{3,1} - T_{5,1}}{2\Delta y}$$

$$T_{5,1} = T_{3,1} - 2\Delta y \frac{\partial T}{\partial y}$$

Substitute into: $T_{4,2} + T_{4,0} + T_{3,1} + T_{5,1} - 4T_{4,1} = 0$

To obtain:

$$T_{4,2} - T_{4,0} + 2T_{3,1} - 2\Delta y \underbrace{\cancel{\frac{\partial T}{\partial y}}}_{\mathbf{0}} - 4T_{4,1} = 0$$

Parabolic PDE's: Finite Difference Solution

Solution of Parabolic PDE's by FD Method

- use B.C.'s and finite difference approximations to formulate the model

- integrate I.C.'s forward through time

- for parabolic systems we will investigate:
  - explicit schemes & stability criteria
  - implicit schemes
    - Simple Implicit
    - Crank-Nicolson (CN)
    - Alternating Direction (A.D.I), 2D-space

Parabolic PDE's: Heat Equation

Prototype problem, Heat Equation (C&C 30.1):

1D $$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2}$$ Find T(x,t)

2D $$\frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$ Find T(x,y,t)

Given the initial temperature distribution

as well as boundary temperatures with

$$k = \frac{k'}{C\rho} = \text{Coefficient of thermal diffusivity}$$

where: $$\begin{cases} k' = \text{coefficient of thermal conductivity} \\ C = \text{heat capacity} \\ \rho = \text{density} \end{cases}$$

Parabolic PDE's: Finite Difference Solution

Solution of Parabolic PDE's by FD Method

1. Discretize the domain into a grid of evenly spaces points (nodes)

2. Express the derivatives in terms of Finite Difference Approximations of $O(h^2)$ and $O(\Delta t)$ [or order $O(\Delta t^2)$]

$$\frac{\partial^2 T}{\partial x^2} \quad \frac{\partial^2 T}{\partial y^2} \quad \frac{\partial T}{\partial t} \longrightarrow \text{Finite Differences}$$

3. Choose $h = \Delta x = \Delta y$, and Δt and use the I.C.'s and B.C.'s to solve the problem by systematically moving ahead in time.

Parabolic PDE's: Finite Difference Solution

Time derivative:

- **Explicit** Schemes (C&C 30.2)

  Express all future ($t + \Delta t$) values, $T(x, t + \Delta t)$, in terms of current (t) and previous ($t - \Delta t$) information, which is known.

- **Implicit** Schemes (C&C 30.3 -- 30.4)

  Express all future ($t + \Delta t$) values, $T(x, t + \Delta t)$, in terms of other future ($t + \Delta t$), current (t), and sometimes previous ($t - \Delta t$) information.

Parabolic PDE's: Notation

Notation:

Use subscript(s) to indicate spatial points.

Use superscript to indicate time level: $T_i^{m+1} = T(x_i, t_{m+1})$

Express a future state, T_i^{m+1}, only in terms of the present state, T_i^m

1-D Heat Equation: $\dfrac{\partial T}{\partial t} = k \dfrac{\partial^2 T}{\partial x^2}$

$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i-1}^m - 2T_i^m + T_{i+1}^m}{(\Delta x)^2} + O(\Delta x)^2 \qquad \text{Centered FDD}$$

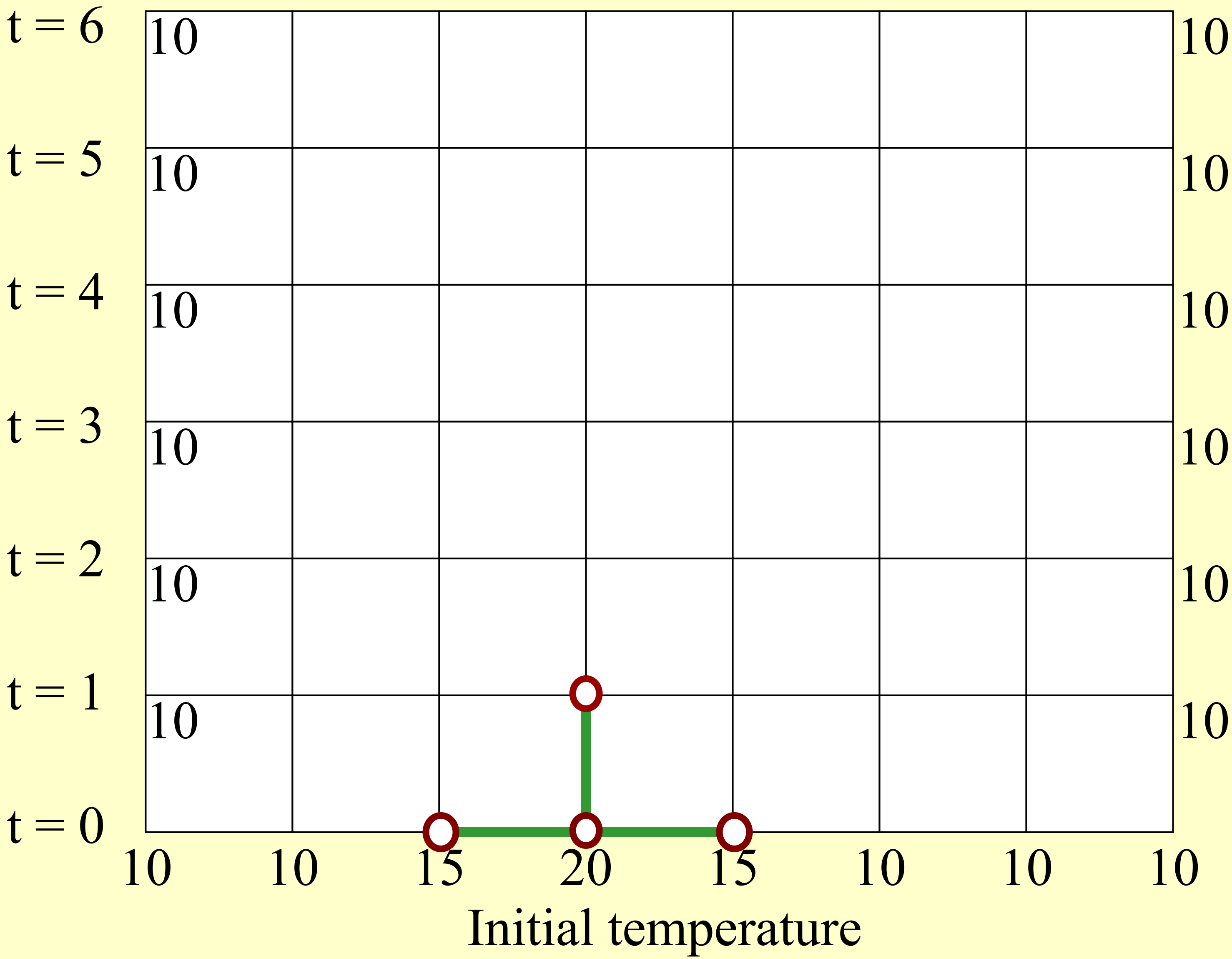
$$\frac{\partial T}{\partial t} = \frac{T_i^{m+1} - T_i^m}{\Delta t} + O(\Delta t) \qquad \text{Forward FDD}$$

Solving for T_i^{m+1} results in:

$$T_i^{m+1} = T_i^m + \lambda(T_{i-1}^m - 2T_i^m + T_{i+1}^m) \quad \text{with } \boldsymbol{\lambda = k\,\Delta t/(\Delta x)^2}$$

$$T_i^{m+1} = (1-2\lambda)\,T_i^m + \lambda\,(T_{i-1}^m + T_{i+1}^m)$$

Parabolic PDE's: Explicit method



Parabolic PDE's: Example - explicit method

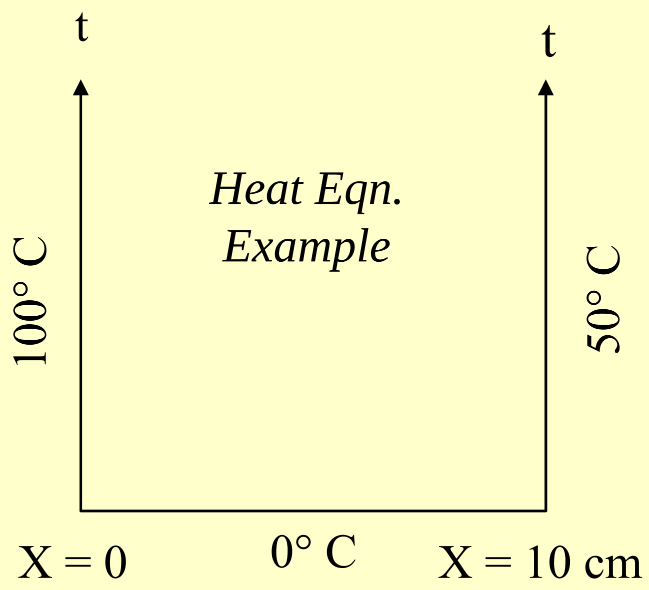
Example: The 1-D Heat Equation $\dfrac{\partial T}{\partial t} = k \dfrac{\partial^2 T}{\partial x^2}$

$k = 0.82$ cal/s·cm·°C, 10-cm long rod,
$\Delta t = 2$ secs, $\Delta x = 2.5$ cm (# segs. = 4)

I.C.'s: $T(0 < x < 10,\ t = 0) = 0°$
B.C.'s: $T(x = 0, \text{all } t) = 100°$
$T(x = 10, \text{all } t) = 50°$

with $\lambda = k\,\Delta t / (\Delta x)^2 = 0.262$

$$\boxed{T_i^{m+1} = T_i^m + \lambda \left(T_{i-1}^m - 2T_i^m + T_{i+1}^m \right)}$$



Parabolic PDE's: Example - explicit method

Example: The 1-D Heat Equation $\dfrac{\partial T}{\partial t} = k\dfrac{\partial^2 T}{\partial x^2}$

$$\boxed{T_i^{m+1} = T_i^m + \lambda\left(T_{i-1}^m - 2T_i^m + T_{i+1}^m\right)}$$

Starting at t = 0 secs. (m = 0), find results at t = 2 secs. (m = 1):

$$T_1^1 = T_1^0 + \lambda(T_0^0 + T_1^0 + T_2^0) = 0 + 0.262[100\text{–}2(0)+0] = 26.2°$$

$$T_2^1 = T_2^0 + \lambda(T_1^0 + T_2^0 + T_3^0) = 0 + 0.262[0\text{–}2(0)+0] = 0°$$

$$T_3^1 = T_3^0 + \lambda(T_2^0 + T_3^0 + T_4^0) = 0 + 0.262[0\text{–}2(0)+50] = 13.1°$$

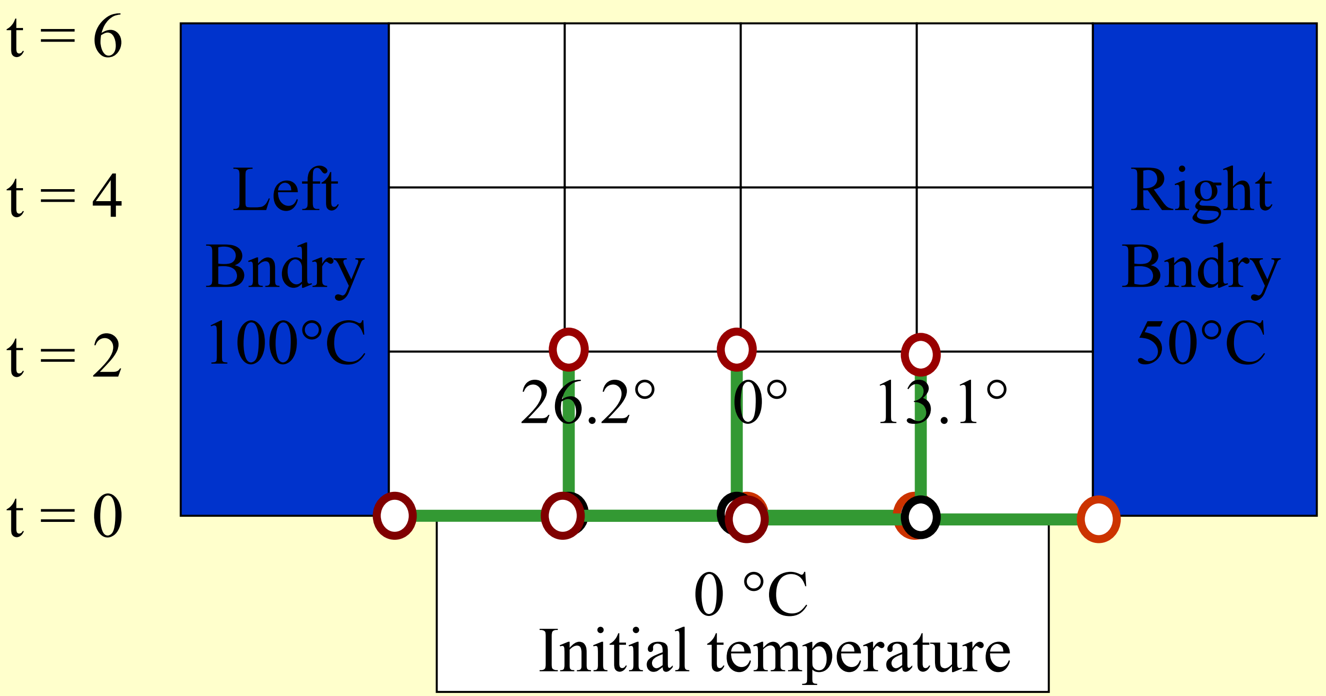
From t = 2 secs. (m = 1), find results at t = 4 secs. (m = 2):

$$T_1^2 = T_1^1 + \lambda(T_0^1 + T_1^1 + T_2^1) = 26.2+0.262[100\text{–}2(26.2)+0] = 38.7°$$

$$T_2^2 = T_2^1 + \lambda(T_1^1 + T_2^1 + T_3^1) = 0+0.262[26.2\text{–}2(0)+13.1] = 10.3°$$

$$T_3^2 = T_3^1 + \lambda(T_2^1 + T_3^1 + T_4^1) = 13.1 + 0.262[0\text{–}2(13.1)+50] = 19.3°$$

Parabolic PDE's: Explicit method

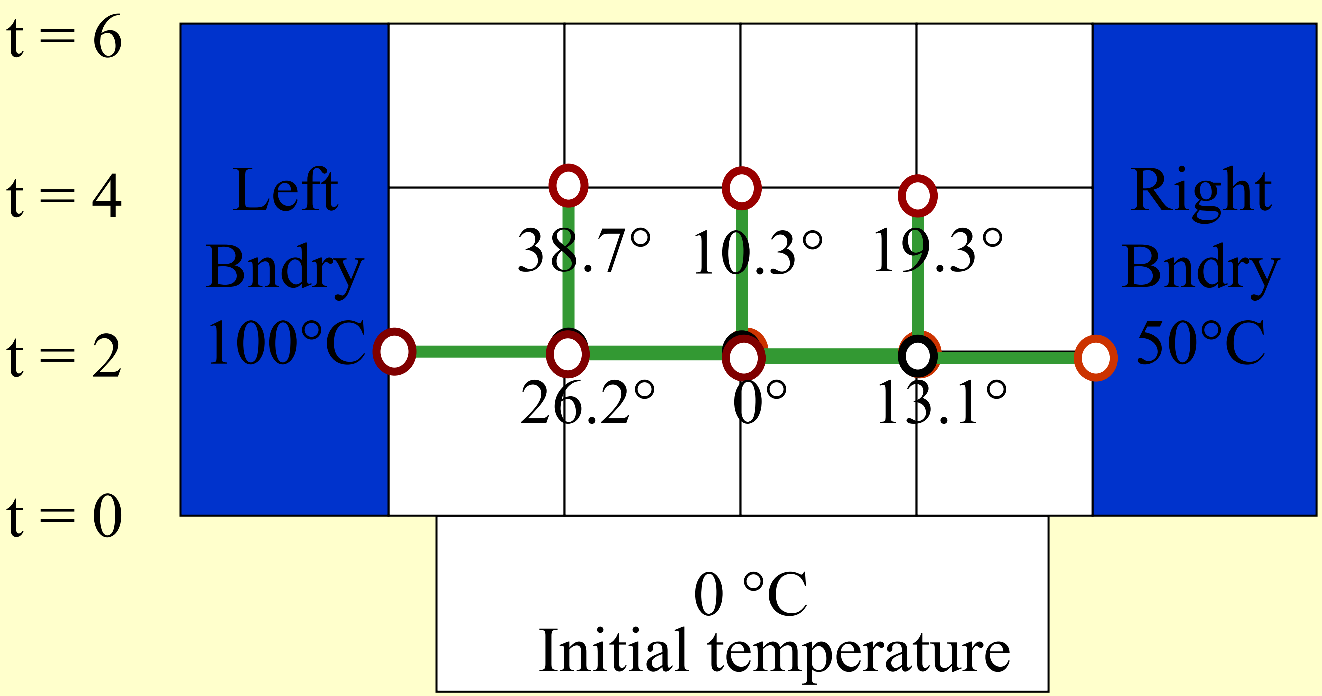


$$T_1^1 = T_1^0 + \lambda(T_0^0 - 2T_1^0 + T_2^0) = 0 + 0.262[100 - 2(0) + 0] = 26.2°$$

$$T_2^1 = T_2^0 + \lambda(T_1^0 - 2T_2^0 + T_3^0) = 0 + 0.262[0 - 2(0) + 0] = 0°$$

$$T_3^1 = T_3^0 + \lambda(T_2^0 - 2T_3^0 + T_4^0) = 0 + 0.262[0 - 2(0) + 50] = 13.1°$$

Parabolic PDE's: Explicit method



$$T_1^2 = T_1^1 + \lambda(T_0^1 - 2T_1^1 + T_2^1) = 26.2 + 0.262[100 - 2(26.2) + 0] = 38.7°$$

$$T_2^2 = T_2^1 + \lambda(T_1^1 - 2T_2^1 + T_3^1) = 0 + 0.262[26.2 - 2(0) + 13.1] = 10.3°$$

$$T_3^2 = T_3^1 + \lambda(T_2^1 - 2T_3^1 + T_4^1) = 13.1 + 0.262[0 - 2(13.1) + 50] = 19.3°$$

Parabolic PDE's: Stability

We will cover stability in more detail later, but we will show that:

The Explicit Method is Conditionally Stable :

For the 1-D spatial problem, the following is the stability condition:

$$\lambda = \frac{k\Delta t}{(\Delta x)^2} \leq \frac{1}{2} \qquad \text{or} \qquad \Delta t \leq \frac{(\Delta x)^2}{2k}$$

$\lambda \leq 1/2$	can still yield oscillation (1D)
$\lambda \leq 1/4$	ensures no oscillation (1D)
$\lambda = 1/6$	tends to optimize truncation error

We will also see that the Implicit Methods are unconditionally stable.

Excel: Explicit

Parabolic PDE's: Explicit Schemes

Summary: Solution of Parabolic PDE's by Explicit Schemes

Advantages: very easy calculations,
simply step ahead

Disadvantage: – low accuracy, $O\ (\Delta t)$
accurate with respect to time
– subject to instability; must use "small" Δt's
➔ requires many steps !!!

Parabolic PDE's: Implicit Schemes

Implicit Schemes for Parabolic PDEs

- Express T_i^{m+1} terms of T_j^{m+1}, T_i^m, and possibly also T_j^m (in which $j = i - 1$ and $i+1$)
- Represents spatial and time domain. For each new time, write m (# of interior nodes) equations and simultaneously solve for m unknown values (banded system).

The 1-D Heat Equation: $$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}$$

Simple Implicit Method. *Substituting:*

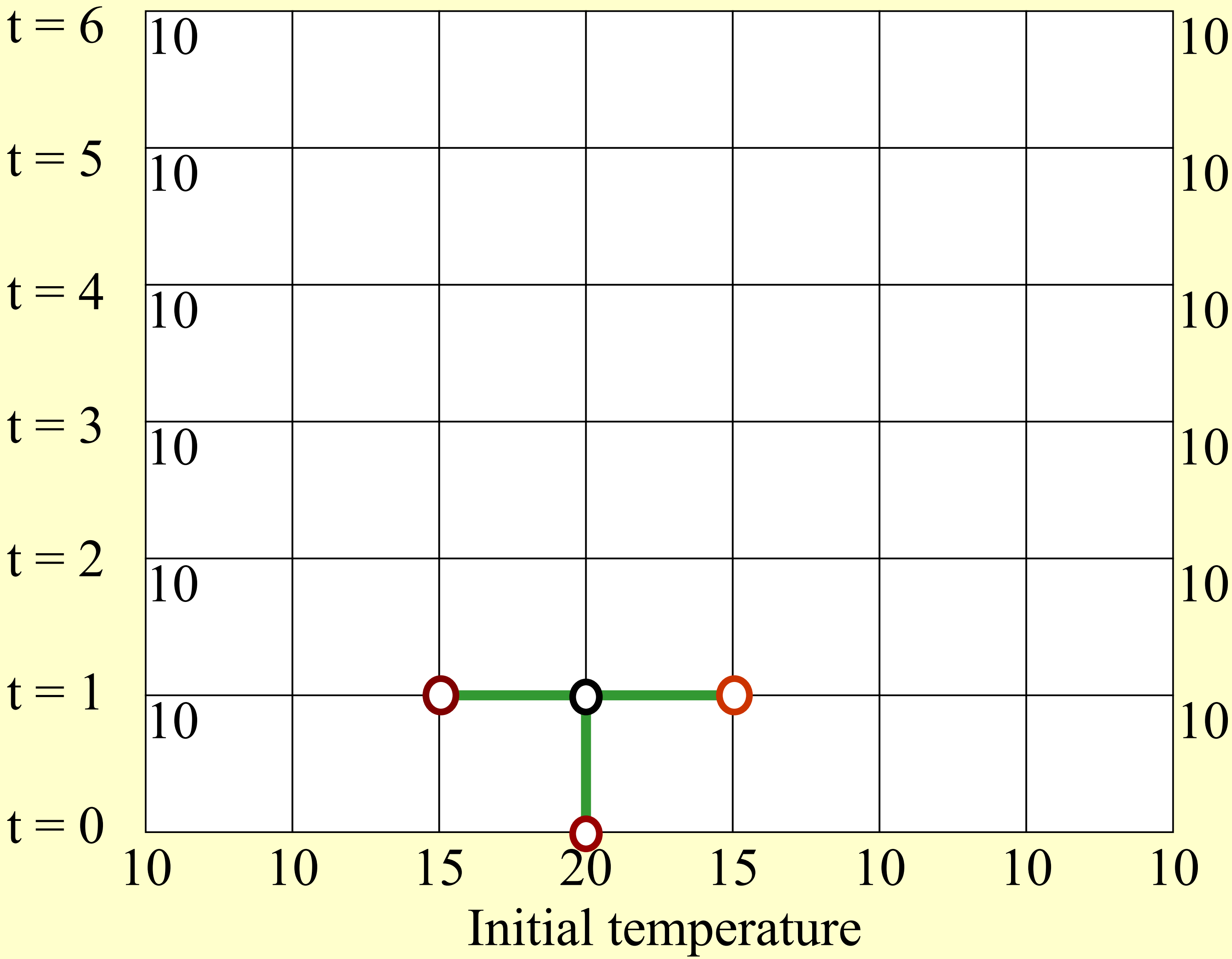
$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{i-1}^{m+1} - 2T_i^{m+1} + T_{i+1}^{m+1}}{(\Delta x)^2} + O(\Delta x)^2 \qquad \text{Centered FDD}$$

$$\frac{\partial T}{\partial t} = \frac{T_i^{m+1} - T_i^m}{\Delta t} + O(\Delta t) \qquad \text{Backward FDD}$$

results in: $-\lambda T_{i-1}^{m+1} + (1+2\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = T_i^m$ with $\lambda = k\dfrac{\Delta t}{(\Delta x)^2}$

1. Requires **I.C.'s** for case where m = 0: i.e., T_i^0 is given for all i.
2. Requires **B.C.'s** to write expressions @ 1st and last interior nodes (i=0 and n+1) for all m.

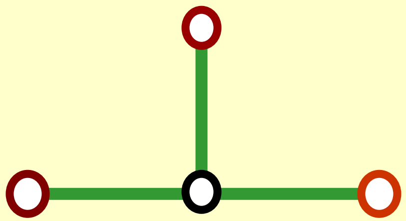
Parabolic PDE's: Simple Implicit Method



Parabolic PDE's: Simple Implicit Method

Explicit Method

m+1



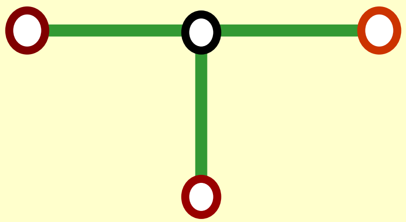
m

i-1 i i+1

$$T_i^{m+1} = T_i^m + \lambda\left(T_{i+1}^m - 2T_i^m + T_{i-1}^m\right)$$

Simple Implicit Method

m +1



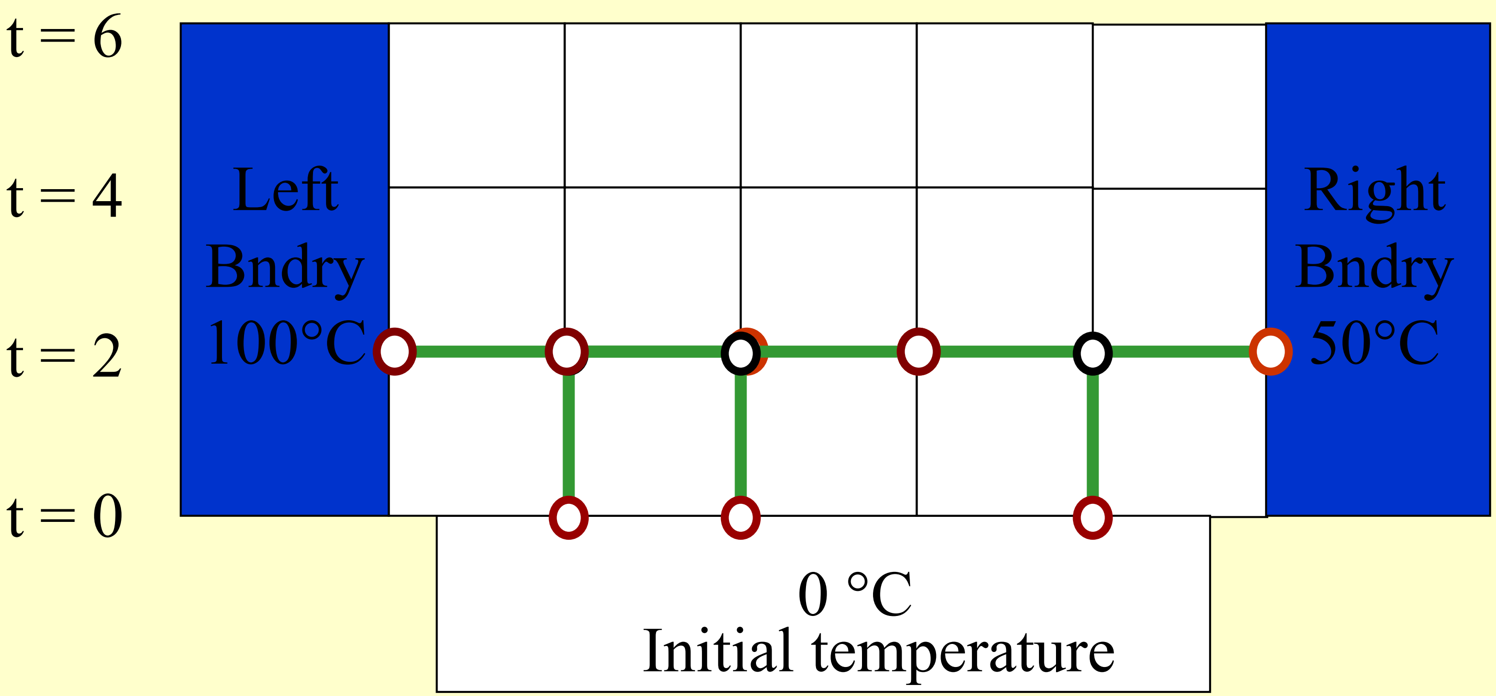
m

i-1 i i+1

$$T_i^m = -\lambda T_{i-1}^{m+1} + \left(1+2\lambda\right)T_i^{m+1} - \lambda T_{i+1}^{m+1}$$

with $\lambda = k\dfrac{\Delta t}{(\Delta x)^2}$ for both

Parabolic PDE's: Simple Implicit Method



At the Left boundary: $(1+2\lambda)T_1^{m+1} - \lambda T_2^{m+1} = T_1^m + \lambda\ T_0^{m+1}$

Away from boundary: $-\lambda T_{i-1}^{m+1} + (1+2\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = T_i^m$

At the Right boundary: $(1+2\lambda)T_i^{m+1} - \lambda T_{i-1}^{m+1} = T_i^m + \lambda\ T_{i+1}^{m+1}$

Parabolic PDE's: Simple Implicit Method

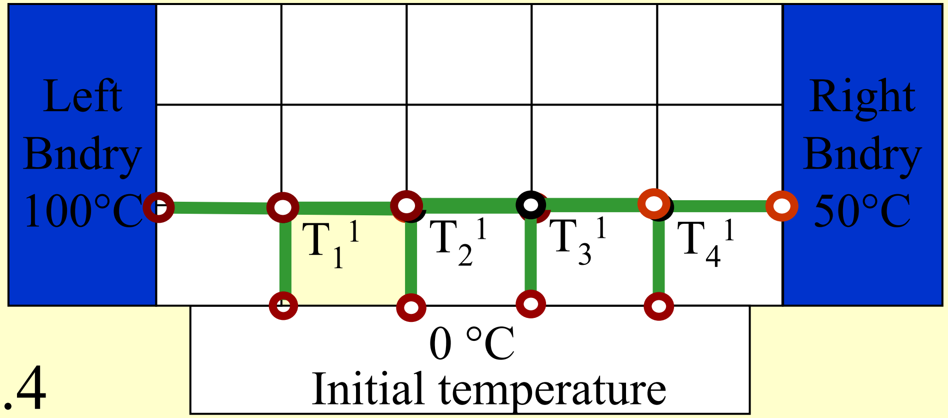
m = 3; t = 6

m = 2; t = 4

m = 1; t = 2

m = 0; t = 0

Let $\lambda = 0.4$



$$\begin{bmatrix} 1.8 & -0.4 & 0 & 0 \\ -0.4 & 1.8 & -0.4 & 0 \\ 0 & -0.4 & 1.8 & -0.4 \\ 0 & 0 & -0.4 & 1.8 \end{bmatrix} \begin{Bmatrix} T_1^1 \\ T_2^1 \\ T_3^1 \\ T_4^1 \end{Bmatrix} = \begin{Bmatrix} 40 \\ 0 \\ 0 \\ 20 \end{Bmatrix}$$

$$\begin{Bmatrix} T_1^1 \\ T_2^1 \\ T_3^1 \\ T_4^1 \end{Bmatrix} = \begin{Bmatrix} 27.6 \\ 6.14 \\ 4.03 \\ 12.0 \end{Bmatrix}$$

At the Left boundary: $(1+2\lambda)T_1^1 - \lambda T_2^1 = T_1^0 + \lambda T_0^1$

$$1.8\, T_1^1 - 0.4\, T_2^1 = 0 + 0.8*100 = \quad 40$$

Away from boundary: $-\lambda T_{i-1}^1 + (1+2\lambda)T_i^1 - \lambda T_{i+1}^1 = T_i^0$

$$-0.4\, T_1^1 + 1.8\, T_2^1 - 0.4\, T_3^1 = 0 = \quad 0$$

$$-0.4\, T_2^1 + 1.8\, T_3^1 - 0.4\, T_4^1 = 0 = \quad 0$$

At the Right boundary: $(1+2\lambda)T_3^1 - \lambda T_2^1 = T_3^0 + \lambda T_4^1$

$$1.8\, T_i^{m+1} - 0.4\, T_{i-1}^{m+1} = 0 + 0.4*50) = \quad 20$$

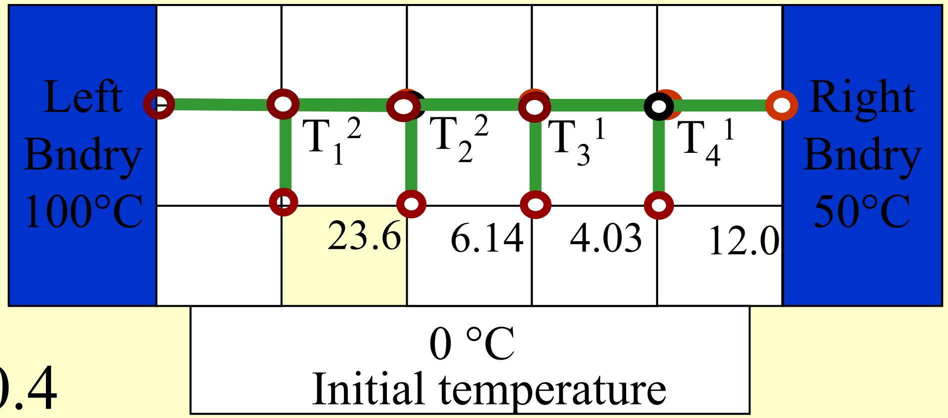
Parabolic PDE's: Simple Implicit Method

m = 3; t = 6

m = 2; t = 4

m = 1; t = 2

m = 0; t = 0



Let $\lambda = 0.4$

$$\begin{bmatrix} 1.8 & -0.4 & 0 & 0 \\ -0.4 & 1.8 & -0.4 & 0 \\ 0 & -0.4 & 1.8 & -0.4 \\ 0 & 0 & -0.4 & 1.8 \end{bmatrix} \begin{Bmatrix} T_1^2 \\ T_2^2 \\ T_3^2 \\ T_4^2 \end{Bmatrix} = \begin{Bmatrix} 78.5 \\ 6.14 \\ 4.03 \\ 32.0 \end{Bmatrix}$$

$$\begin{Bmatrix} T_1^2 \\ T_2^2 \\ T_3^2 \\ T_4^2 \end{Bmatrix} = \begin{Bmatrix} 38.5 \\ 14.1 \\ 9.83 \\ 20.0 \end{Bmatrix}$$

At the Left boundary: $(1+2\lambda)T_1^2 - \lambda T_2^2 = T_1^1 + \lambda T_0^2$

$$1.8\, T_1^2 - 0.4\, T_2^2 = 23.6 + 0.4*100 = \quad 78.5$$

Away from boundary: $-\lambda T_{i-1}^2 + (1+2\lambda)T_i^2 - \lambda T_{i+1}^2 = T_i^1$

$$-0.4*T_1^2 + 1.8*T_2^2 - 0.4*T_3^2 = 6.14 = \quad 6.14$$

$$-0.4*T_2^2 + 1.8*T_3^2 - 0.4*T_4^2 = 4.03 = \quad 4.03$$

At the Right boundary: $(1+2\lambda)T_3^2 - \lambda T_4^2 = T_3^1 + \lambda T_4^2$

$$1.8*T_3^2 - 0.4*T_4^2 = 12.0 + 0.4*50 = \quad 32.0$$

Excel: Implicit

Parabolic PDE's: Crank-Nicolson Method

Implicit Schemes for Parabolic PDEs

Crank-Nicolson (CN) Method (Implicit Method)

Provides 2nd-order accuracy in both space and time.

Average the 2nd-derivative in space for t^{m+1} and t^m.

$$\frac{\partial^2 T}{\partial x^2} = \frac{1}{2}\left[\frac{T_{i-1}^{m} - 2T_i^{m} + T_{i+1}^{m}}{(\Delta x)^2} + \frac{T_{i-1}^{m+1} - 2T_i^{m+1} + T_{i+1}^{m+1}}{(\Delta x)^2}\right] + O(\Delta x)^2$$

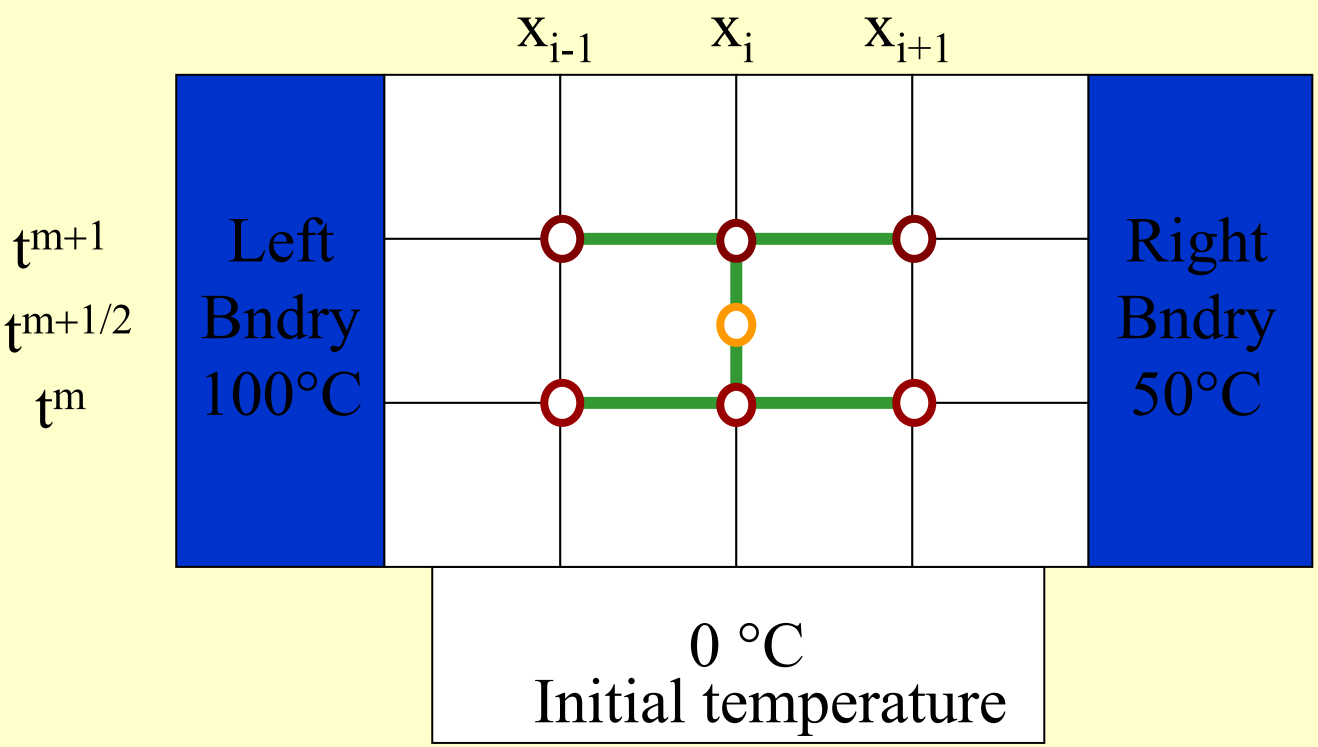
$$\frac{\partial T}{\partial t} = \frac{\mathbf{T}_i^{m+1} - T_i^{m}}{\Delta t} + O(\Delta t^2) \quad \text{(central difference in time now)}$$

$$-\lambda T_{i-1}^{m+1} + 2(1+\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = \lambda T_{i-1}^{m} + 2(1-\lambda)T_i^{m} - \lambda T_{i+1}^{m}$$

Requires I.C.'s for case where m = 0: T_i^0 = given value, f(x)

Requires B.C.'s in order to write expression for T_0^{m+1} & T_{i+1}^{m+1}

Parabolic PDE's: Crank-Nicolson Method



$$-\lambda T_{i-1}^{m+1} + 2(1+\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = \lambda T_{i-1}^{m} + 2(1-\lambda)T_i^{m} - \lambda T_{i+1}^{m}$$

Crank-Nicolson

Parabolic PDE's: Implicit Schemes

Summary: Solution of Parabolic PDE's by Implicit Schemes

Advantages:

- Unconditionally stable.
- Δt choice governed by overall accuracy.
  [Error for CN is $O(\Delta t^2)$]
- May be able to take larger Δt ➔ fewer steps

Disadvantages:

- More difficult calculations,
  especially for 2D and 3D spatially
- For 1D spatially, effort $\approx$ same as explicit
  because system is tridiagonal.

Stability Analysis of Numerical Solution to Heat Eq.

Consider the classical solution of the Heat Equation:

$$\frac{\partial T}{\partial t} = k\frac{\partial^2 T}{\partial x^2}$$

To find the form of the solutions, try:

$$T(x,t) = e^{-at}\sin(\omega x)$$

Substituting this into the Heat Equation yields:

$$- a\, T(x,t) = - k\, \omega^2\, T(x,t)$$

OR $$a = k\,\omega^2$$

$$\Rightarrow \quad T(x,t) = e^{-k\omega^2 t}\sin(\omega x)$$

Each sin component of the initial temperature distribution **decays** as

$$\exp\{- k\,\omega^2\, t)$$

Stability Analysis

Consider FD schemes as advancing one step with a "transition equation":

$$\{\mathbf{T}^{m+1}\} = [\mathbf{A}]\ \{\mathbf{T}^{m}\} \qquad \text{with } [A] \text{ a function of } \lambda = k\ \Delta t\ /\ (\Delta x)^2$$

$$\text{with} \quad \left\{T^m\right\} = \left\lfloor T_1^m, T_2^m, \ldots, T_i^m, \ldots, T_n^m \right\rfloor^T$$

with zero boundary conditions

First step can be written:

$$\{T^1\} = [A]\ \{T^0\} \qquad \text{w/ } \{T^0\} = \text{initial conditions}$$

Second step as:

$$\{T^2\} = [A]\ \{T^1\} = [A]^2\{T^0\}$$

and m^{th} step as:

$$\{T^m\} = [A]\ \{T^{m-1}\} = [A]^m\{T^0\}$$

(Here "m" is an exponent on [A])

Stability Analysis

$$\{T^m\} = [A]^m\{T^0\}$$

- For the influence of the initial conditions and any rounding errors in the IC (or rounding or truncation errors introduced in the transition process) to decay with time, it must be the case that $\| A \| < 1.0$

- If $\| A \| > 1.0$, some eigenvectors of the matrix [A] can grow without bound generating ridiculous results. In such cases the method is said to be **unstable.**

- Taking $r = \| A \| = \| A \|_2$ = maximum eigenvalue of [A] for symmetric A (the "spectral norm"), the maximum eigenvalue describes the **stability** of the method.

Stability Analysis

Illustration of Instability of Explicit Method (for a simple case)

Consider 1D spatial case: $T_i^{m+1} = \lambda T_{i-1}^{m} + (1-2\lambda)T_i^{m} + \lambda T_{i+1}^{m}$

Worst case solution: $T_i^{m} = r^{m}(-1)^{i}$ (high frequency x-oscillations in index i)

Substitution of this solution into the difference equation yields:

$$r^{m+1}(-1)^{i} = \lambda\, r^{m}(-1)^{i-1} + (1-2\lambda)\, r^{m}(-1)^{i} + \lambda\, r^{m}(-1)^{i+1}$$

$$r = \lambda(-1)^{-1} + (1-2\lambda) + \lambda(-1)^{+1}$$

or $\boldsymbol{r = 1 - 4\lambda}$

If initial conditions are to decay and nothing "explodes," we need:

$-1 < r < 1$ or $0 < \lambda < 1/2.$

For no oscillations we want:

$0 < r < 1$ or $0 < \lambda < 1/4.$

Stability of the Simple Implicit Method

Consider 1D spatial: $-\lambda T_{i-1}^{m+1} + (1+2\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = T_i^m$

Worst case solution: $T_i^m = r^m \left(-1\right)^i$

Substitution of this solution into difference equation yields:

$$-\lambda r^{m+1}\left(-1\right)^{i-1} + \left(1-2\lambda\right) r^{m+1}\left(-1\right)^{i} - \lambda r^{m+1}\left(-1\right)^{i+1} = r^m\left(-1\right)^i$$

$$r\,[-\lambda\,(-1)^{-1} + (1+2\lambda) - \lambda\,(-1)^{+1}] = 1$$

or **$r = 1/[1 + 4\lambda]$**

i.e., $0 < r < 1$ for all $\lambda > 0$

Stability of the Crank-Nicolson Implicit Method

Consider:

$$-\lambda T_{i-1}^{m+1} + 2(1+\lambda)T_i^{m+1} - \lambda T_{i+1}^{m+1} = \lambda T_{i-1}^{m} + 2(1-\lambda)T_i^{m} + \lambda T_{i+1}^{m}$$

Worst case solution: $T_i^m = r^m(-1)^i$

Substitution of this solution into difference equation yields:

$$-\lambda r^{m+1}(-1)^{i-1} + 2(1+\lambda)r^{m+1}(-1)^{i} - \lambda r^{m+1}(-1)^{i+1} =$$

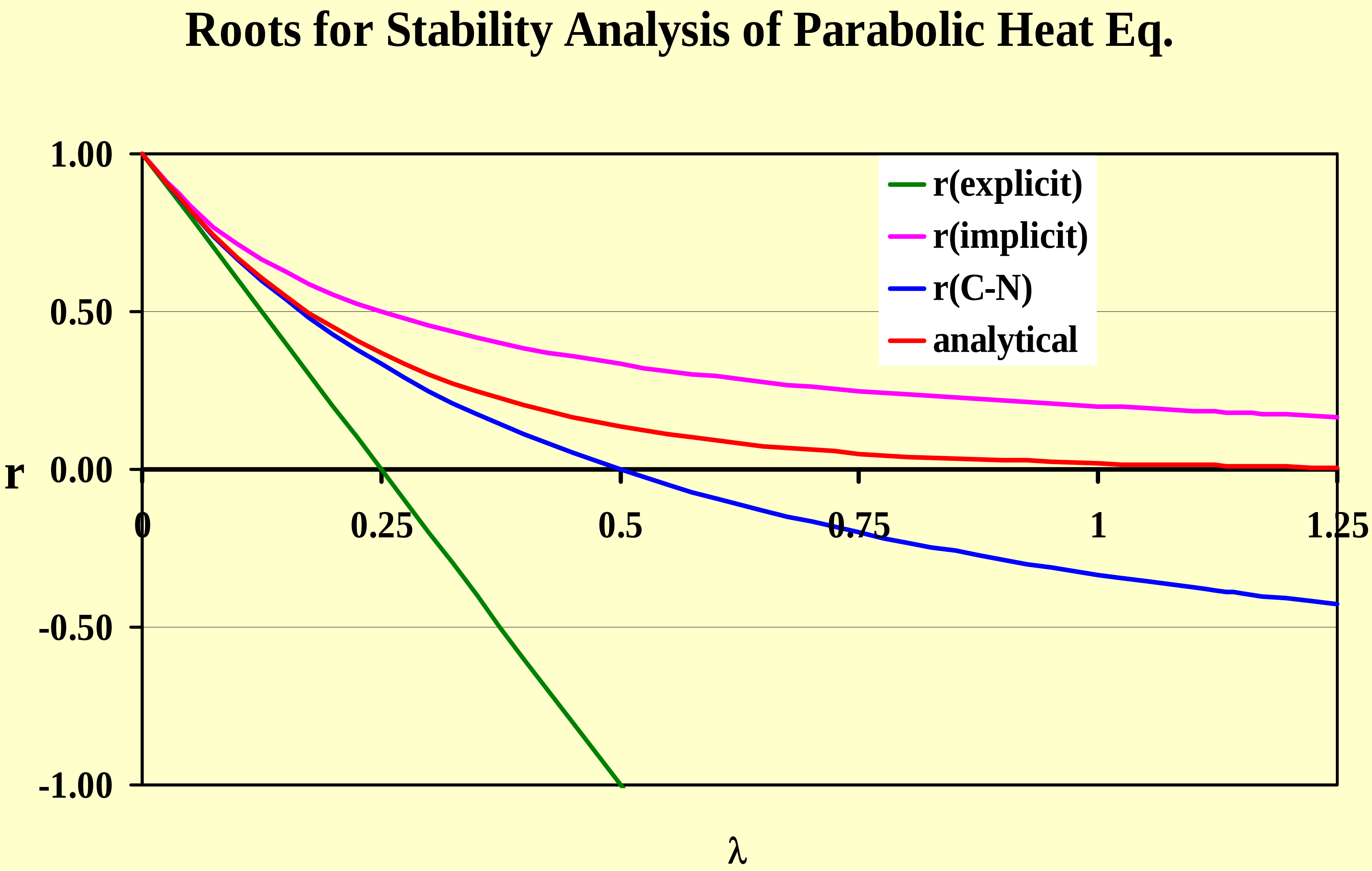
$$\lambda r^{m}(-1)^{i-1} + 2(1-\lambda)r^{m}(-1)^{i} + \lambda r^{m}(-1)^{i+1}$$

$$r\,[-\lambda\,(-1)^{-1} + 2(1+\lambda) - \lambda\,(-1)^{+1}] = \lambda\,(-1)^{-1} + 2(1-\lambda) + \lambda\,(-1)^{+1}$$

or $\quad$ $\mathbf{r = [1 - 2\lambda] / [1 + 2\lambda]}$

i.e., $\quad$ $|\,r\,| < 1$ for all $\lambda > 0$

Stability Summary, Parabolic Heat Equation



Parabolic PDE's: Stability

Implicit Methods are <u>Unconditionally Stable</u> :

Magnitude of **all** eigenvalues of [A] is < 1 for **all** values of λ.

➔ Δx and Δt can be selected solely to control the **overall** accuracy.

Explicit Method is <u>Conditionally Stable</u> :

Explicit, 1-D Spatial: $\lambda = \dfrac{k\Delta t}{(\Delta x)^2} \le \dfrac{1}{2}$ or $\Delta t \le \dfrac{(\Delta x)^2}{2k}$

$\lambda \le 1/2$	can still yield oscillation (1D)
$\lambda \le 1/4$	ensures no oscillation (1D)
$\lambda = 1/6$	tends to optimize truncation error

Explicit, 2-D Spatial: $\lambda = \dfrac{k\Delta t}{h^2} \le \dfrac{1}{4}$ or $\Delta t \le \dfrac{h^2}{4k}$

$(h = \Delta x = \Delta y)$

Parabolic PDE's in Two Spatial dimension

2D $$\frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right)$$ Find T(x,y,t)

Explicit solutions :

Stability criterion $$\Delta t \le \frac{(\Delta x)^2 + (\Delta y)^2}{8k}$$

if $h = \Delta x = \Delta y$ ==> $$\lambda = \frac{k\Delta t}{h^2} \le \frac{1}{4} \quad \text{or} \quad \Delta t \le \frac{h^2}{4k}$$

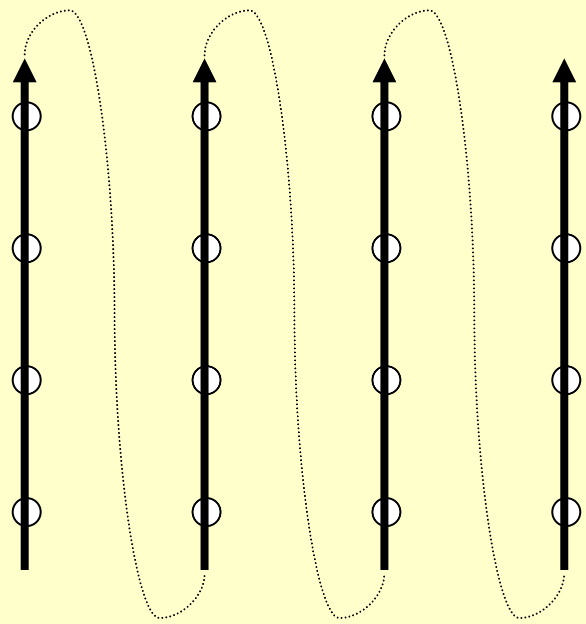
Implicit solutions : No longer tridiagonal

Parabolic PDE's: ADI method

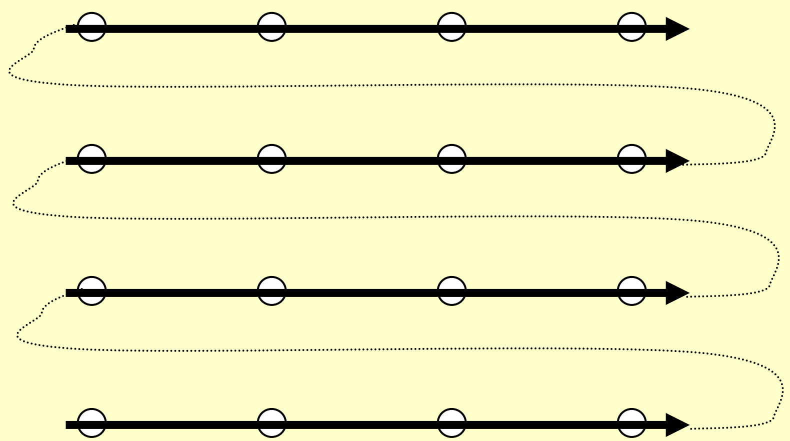
Alternating-Direction Implicit (ADI) Method

- Provides a method for using ***tridiagonal*** matrices for solving parabolic equations in 2 spatial dimensions.

- Each time increment is implemented in two steps:



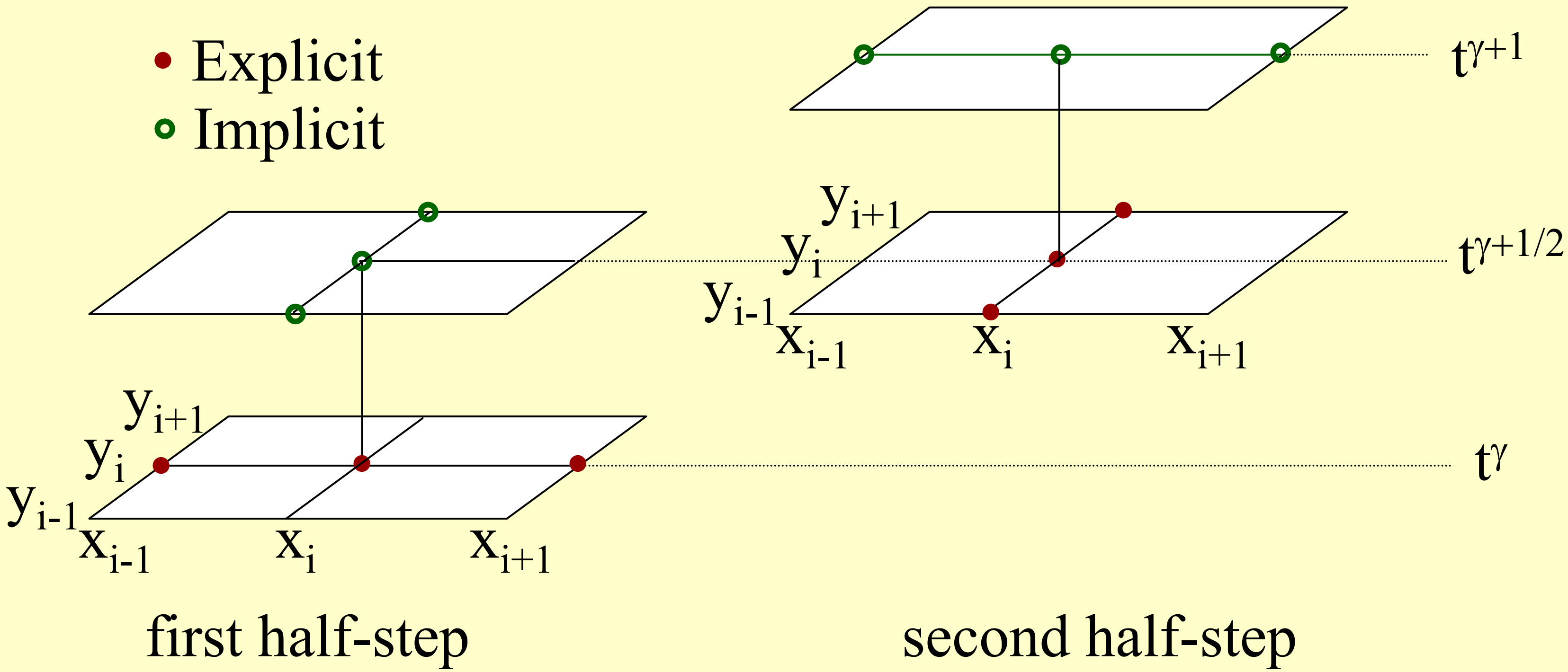
first direction



second direction

Parabolic PDE's: ADI method

- Provides a method for using ***tridiagonal*** matrices for solving parabolic equations in 2 spatial dimensions.
- Each time increment is implemented in two steps:



ADI example