# Topics

Nonlinear Equations

Analysis of PDEs

Elliptic PDEs & Boundary-Value ODEs

Parabolic PDEs & Initial Value ODEs

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# Nonlinear Equations

CHEN 6603

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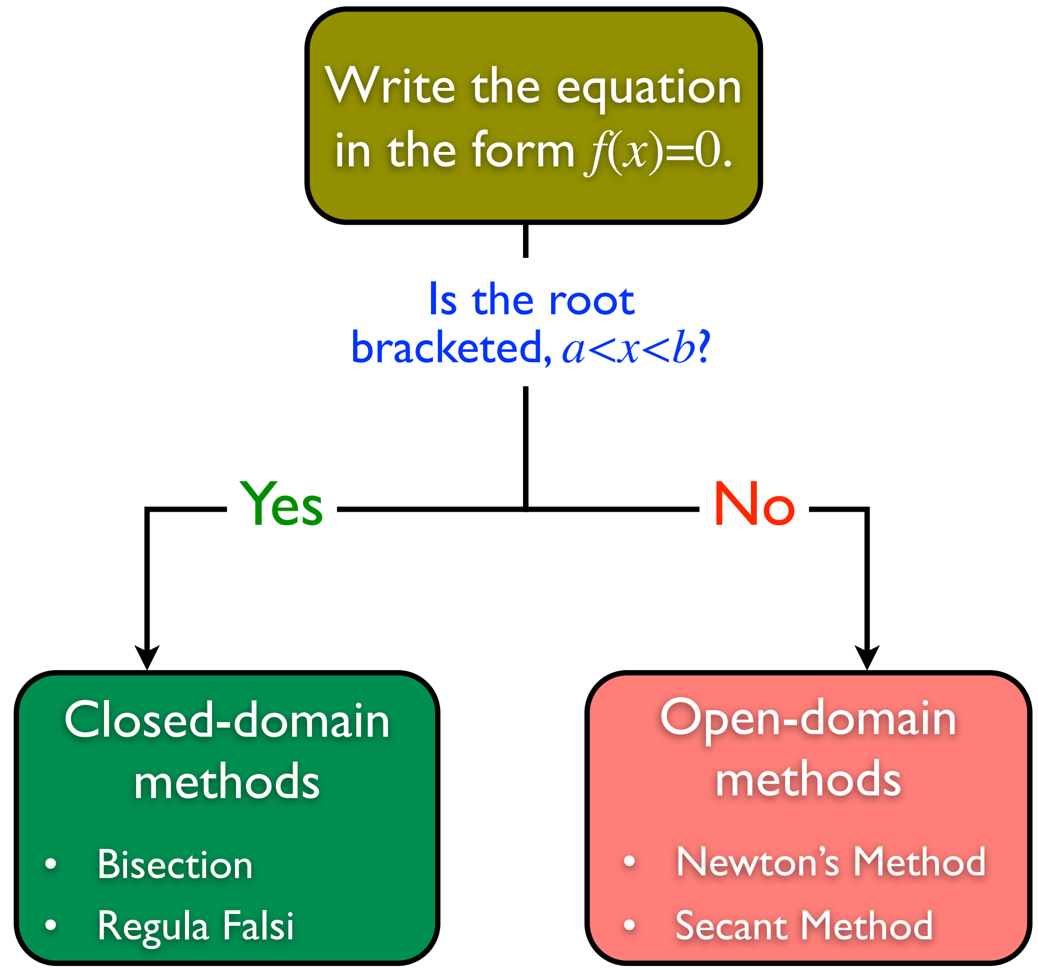
# Nonlinear Eqns. - Overview

## Characteristics:

- May have 0 ... many solutions
- Solution methods are *iterative* and require an *initial guess* for the solution.
- Not guaranteed to find the solution, even if one exists!
  - Initial guess can be critical to finding the solution.
  - Bad initial guess may lead to no convergence, or convergence to a wrong (unintended) root.
- Solve for *roots*, $f(x)=0$. If you want $f(x)=a$, then write in residual form, $r(x)=f(x)-a$ and solve $r(x)=0$.

## Solution Approaches

- Closed-Domain Methods
  - Bracket the root and "home in" on it.
  - Quite simple & robust, but require you to bound the root.
  - Can be problematic if you bound multiple roots...
- Open Domain Methods
  - Require an initial guess for the solution, but not a bracket.
  - More efficient, but less robust than closed-domain methods.



# Nonlinear Systems - Newton's Method

$$\mathbf{f}(\mathbf{x}) = 0 \quad \Longleftrightarrow \quad \begin{pmatrix} f_1(x_1, x_2, \cdots, x_n) \\ f_2(x_1, x_2, \cdots, x_n) \\ \vdots \\ f_n(x_1, x_2, \cdots, x_n) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$\mathbf{x}$ is a vector of unknowns.

Taylor Series expansion of $f_i$ in terms of $\mathbf{x}$:

$$f_i(\mathbf{x}) \approx f_i(\mathbf{x}_0) + \sum_{j=1}^{n} \underbrace{\frac{\partial f_i}{\partial x_j}}_{J_{ij}} \underbrace{(x_j - x_{j0})}_{\Delta x_j} + \mathcal{O}(\Delta x^2)$$

Example: $n$=2 equations:

$$\begin{aligned} f_1(x_1, x_2) &= f_1(x_{1,0}, x_{2,0}) + \frac{\partial f_1}{\partial x_1}(x_1 - x_{1,0}) + \frac{\partial f_1}{\partial x_2}(x_2 - x_{2,0}) \\ f_2(x_1, x_2) &= f_2(x_{1,0}, x_{2,0}) + \frac{\partial f_2}{\partial x_1}(x_1 - x_{1,0}) + \frac{\partial f_2}{\partial x_2}(x_2 - x_{2,0}) \end{aligned}$$

$\mathbf{f}(\mathbf{x}) \approx \mathbf{f}(\mathbf{x}_0) + \mathbf{J}\Delta\mathbf{x}$ $\quad \Delta\mathbf{x}$ is a vector of corrections (updates).

$$\mathbf{J} = \begin{bmatrix} \frac{\partial f_1(\mathbf{x}_0)}{\partial x_1} & \frac{\partial f_1(\mathbf{x}_0)}{\partial x_2} & \cdots & \frac{\partial f_1(\mathbf{x}_0)}{\partial x_n} \\ \frac{\partial f_2(\mathbf{x}_0)}{\partial x_1} & \frac{\partial f_2(\mathbf{x}_0)}{\partial x_2} & \cdots & \frac{\partial f_2(\mathbf{x}_0)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_n(\mathbf{x}_0)}{\partial x_1} & \frac{\partial f_n(\mathbf{x}_0)}{\partial x_2} & \cdots & \frac{\partial f_n(\mathbf{x}_0)}{\partial x_n} \end{bmatrix}$$

We want solution at $f(\mathbf{x})$=0. Therefore:

Newton's Method

$$\mathbf{J}\Delta\mathbf{x} = -\mathbf{f}(\mathbf{x}_0)$$

This is a *linear* system of equations!

## Algorithm

Given $f(\mathbf{x})$, $\mathbf{x}_0$, $\mathbf{J}$.

1. Calculate $[\mathbf{J}]$ & $f(\mathbf{x})$ at the current guess for $(\mathbf{x})$.
2. Solve for $(\Delta\mathbf{x})$
3. Update $x_i$
4. If not converged, go to 1.

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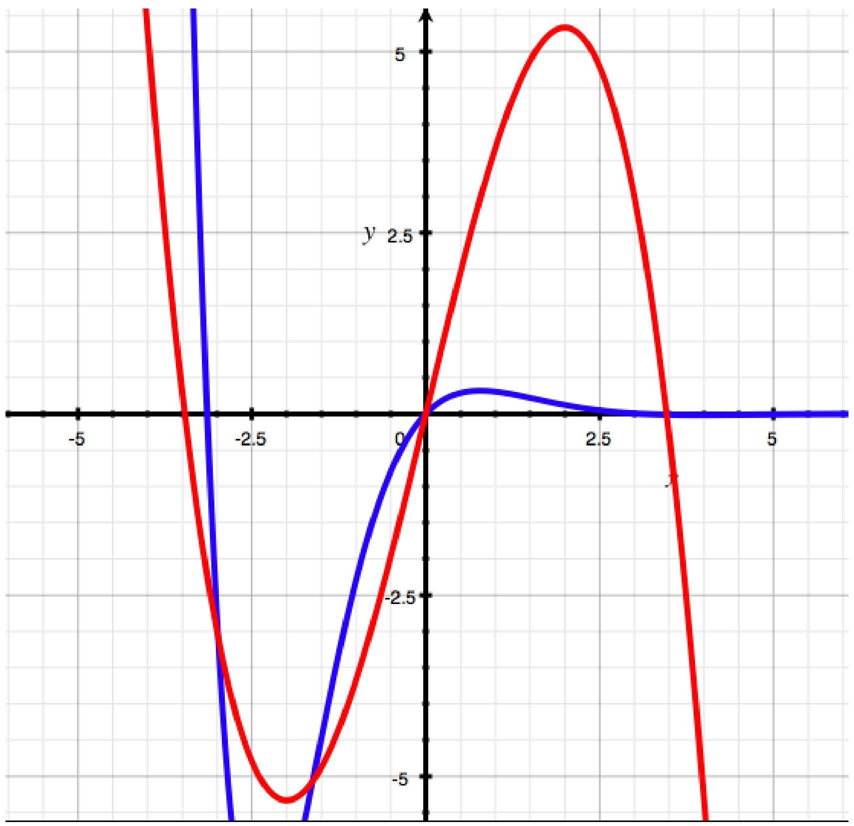
# Newton's Method - Example




Original Equations: $$\frac{1}{2}x^3 + y = 4x$$
$$y = \sin(x)\exp(-x)$$

Modified Equations: $$\begin{aligned} f_1 &= \frac{1}{2}x^3 + y - 4x \\ f_2 &= y - \sin(x)\exp(-x) \end{aligned}$$

Jacobian: $$[J] = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix} = \begin{bmatrix} \frac{3}{2}x^2 - 4 & 1 \\ -\cos(x)\exp(-x) + \sin(x)\exp(-x) & 1 \end{bmatrix}$$

# Example - cont'd

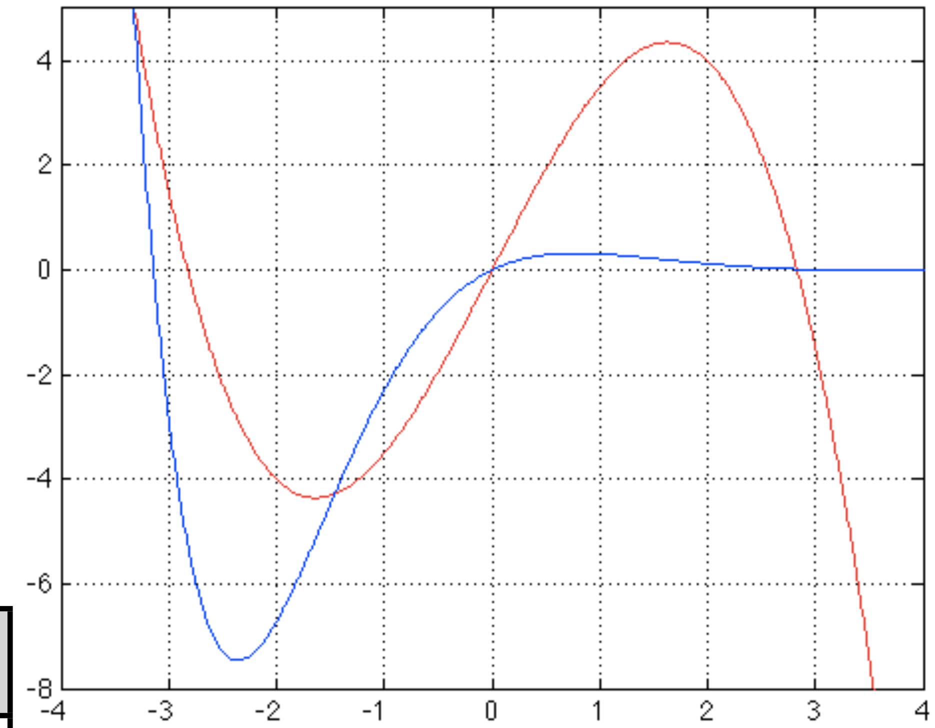
$$f_1 = \frac{1}{2}x^3 + y - 4x$$
$$f_2 = y - \sin(x)\exp(-x)$$

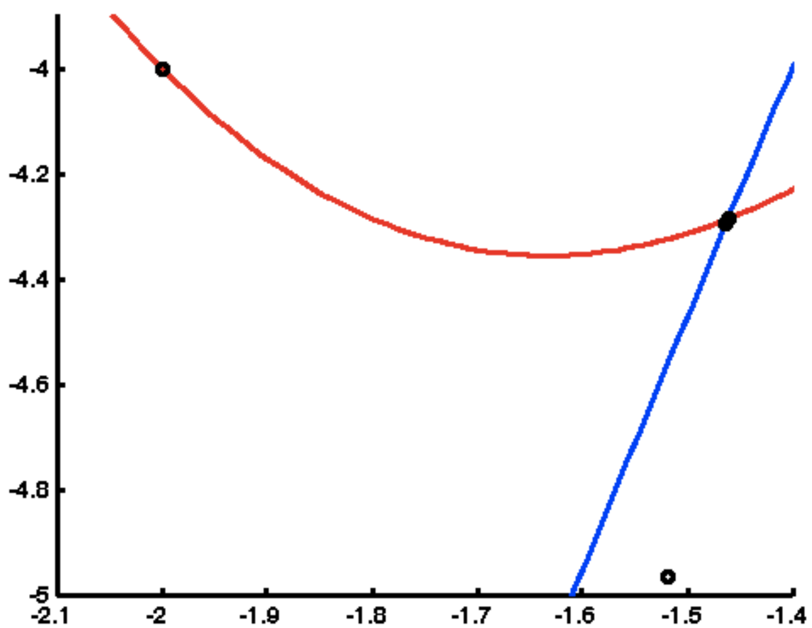
1. Guess $x_i$: $x = -2, \quad y = -4$

2. Calculate $[J]$ & $(f)$ $[J] = \begin{bmatrix} 2.0 & 1 \\ -3.6439 & 1 \end{bmatrix} \qquad (f) = \begin{pmatrix} 0.0 \\ 2.7188 \end{pmatrix}$

3. Solve for $(\Delta)$ $(\Delta) = \begin{pmatrix} 0.4817 \\ -0.9635 \end{pmatrix}$

4. Update $x_i$ $x = -1.5183, \quad y = -4.9635$




| $k$ | $x$ | $y$ |
|---|---|---|
| 0 | -2 | -4 |
| 1 | -1.5183 | -4.9635 |
| 2 | -1.4631 | -4.2932 |
| 3 | -1.4611 | -4.2848 |
| 4 | -1.4611 | -4.2848 |

# Software Tools

Must provide a function to evaluate the residual.

- MATLAB
  - FZERO - good for single nonlinear equation, solves for $x$ such that $f(x)=0$.
  - FSOLVE - for systems of nonlinear equations, finds $x_i$ such that $f_j(x_i)=0$.
    - requires the "optimization toolbox"
  - FMINSEARCH - good for systems of nonlinear equations
    - Searches for the minimum, not the zeros.
- Excel
  - Goal Seek - single variable
  - Solver - multiple variables

Solve the last problem again in MATLAB…

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# Analysis of PDEs

3-D rectangular coordinate system: $\nabla = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}$

**PDEs**

$$\rho c_p \frac{\partial T}{\partial t} = -\rho c_p \mathbf{u} \cdot \nabla T + \frac{\partial p}{\partial t} + \mathbf{u} \cdot \nabla p + \boldsymbol{\tau} : \nabla \mathbf{u} - \nabla \cdot \mathbf{q} + s_T$$

- Time-rate of change in $T$ at a point in space.
- Convection of $T$ (velocity pushing it around)
- $T$ changes due to changes in $p$.
- $T$ changes due to viscous heating.
- $T$ changes due to thermal & species diffusion.
- $T$ changes from other sources (reaction, radiation, etc).

Solution

Algebraic Equations

Assumptions

Solution

Assume:

1. Velocity is zero.
2. Pressure is constant.
3. Steady-state.
4. $\mathbf{q} = -\lambda \nabla T$ (Fourier's Law of conduction)
5. $\lambda$ is constant.
6. One-dimensional

Assume:

1. Velocity is zero.
2. Pressure is constant.
3. $T$ does not vary spatially.
4. $s_T = -hA/V\,(T - T_\infty)$

**ODEs**

$$\frac{\mathrm{d}^2 T}{\mathrm{d}x^2} = -\frac{s_T}{\lambda}$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -\frac{hA}{\rho c_p V}(T - T_\infty)$$

# Numerical Solutions to PDEs

- For systems which have a time derivative ($\partial \phi / \partial t$)
  - Convert the PDE into a system of ODEs
    - Method of Lines: "Discretize" in space. Then we are left with a system of ODEs.
    - Number of ODEs is dependent on spatial discretization.

$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} + s_\phi$$

"Parabolic" PDE

- For PDEs which do not have a time derivative (Elliptic PDEs):
  - Called "boundary value problems"
  - Convert to a big system of (nonlinear) equations.
  - Number of equations depends on spatial discretization (next).

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\frac{s_\phi}{D_\phi}$$

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# Elliptic PDEs

Here we will show examples primarily for Boundary-Value ODEs

Elliptic PDE: $$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\frac{s_\phi}{D_\phi}$$

Boundary value ODE: $$\frac{\mathrm{d}^2 \phi}{\mathrm{d}x^2} = -\frac{s_\phi}{D_\phi}$$

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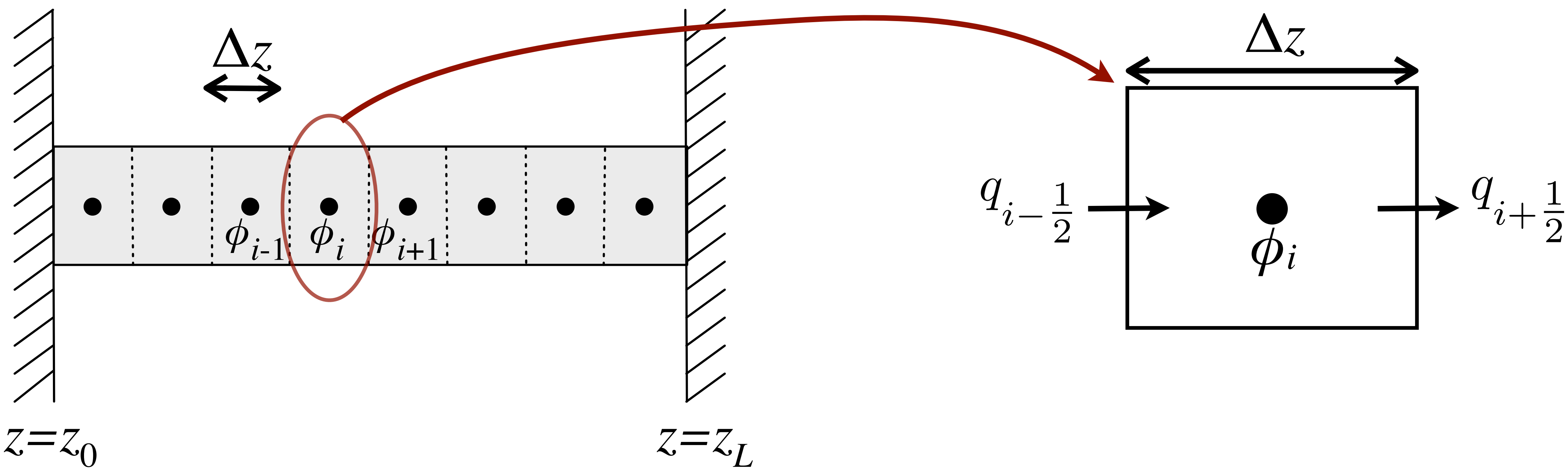
# Discrete Calculus (1-D)




$$\left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{i+\frac{1}{2}} = \frac{\phi_{i+1} - \phi_i}{\Delta z} + \mathcal{O}(\Delta z^2)$$

Approximation for the derivative of $\phi$ at the midpoint of two points.

Assume a flux, $q$, of the form:

$$q = -D\frac{\mathrm{d}\phi}{\mathrm{d}z}$$

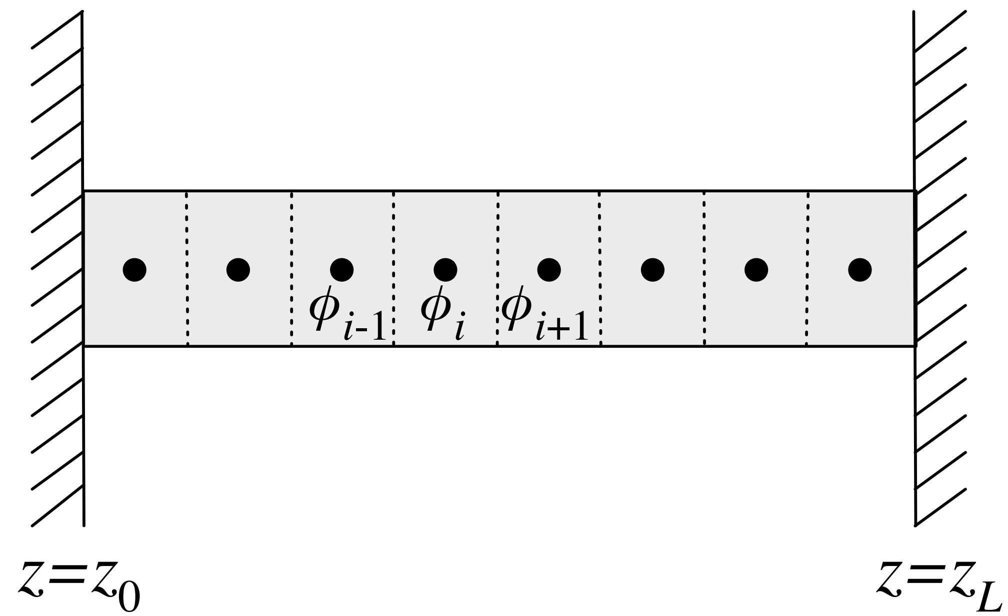
We may approximate $q$ as:

$$q_{i+\frac{1}{2}} \approx -D_{i+\frac{1}{2}} \frac{\phi_{i+1} - \phi_i}{\Delta z}$$

$$q_{i-\frac{1}{2}} \approx -D_{i-\frac{1}{2}} \frac{\phi_i - \phi_{i-1}}{\Delta z}$$

# Second Derivatives

$$\left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{i+\frac{1}{2}} = \frac{\phi_{i+1}-\phi_i}{\Delta z} + \mathcal{O}(\Delta z^2)$$




Use the same approximation on the *derivatives* of $\phi$ to obtain:

$$\begin{aligned}\left.\frac{\mathrm{d}^2\phi}{\mathrm{d}z^2}\right|_i &= \frac{\left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{i+\frac{1}{2}} - \left.\frac{\mathrm{d}\phi}{\mathrm{d}z}\right|_{i-\frac{1}{2}}}{\Delta z} + \mathcal{O}(\Delta z^2), \\ &= \frac{1}{\Delta z}\left[\frac{\phi_{i+1}-\phi_i}{\Delta z} - \frac{\phi_i-\phi_{i-1}}{\Delta z}\right] + \mathcal{O}(\Delta z^2)\end{aligned}$$

$$\boxed{\left.\frac{\mathrm{d}^2\phi}{\mathrm{d}z^2}\right|_i = \frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{\Delta z^2} + \mathcal{O}(\Delta z^2)}$$

Approximation for the second derivative, valid for uniformly spaced cells.

# Example - Steady Diffusion

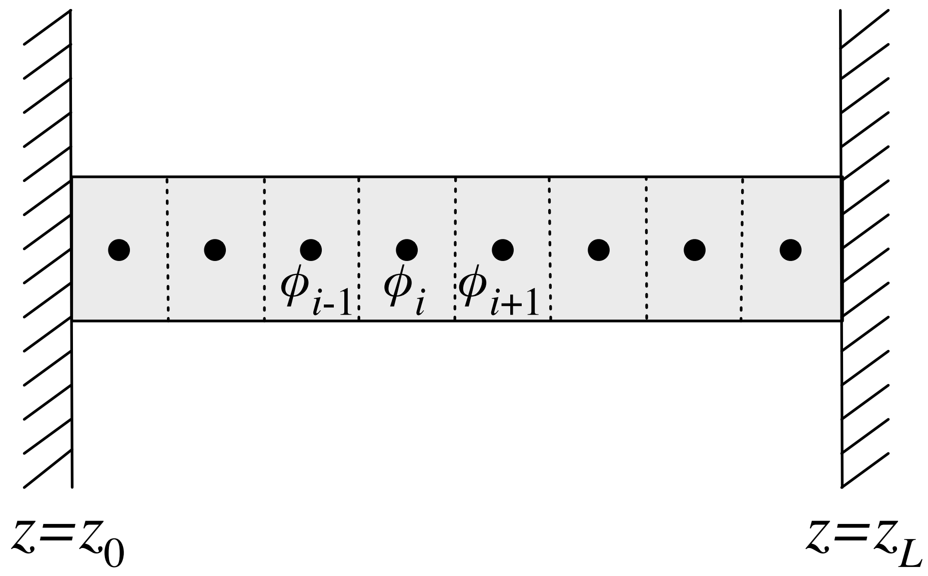
Steady state, no convection: $\nabla \cdot \mathbf{q} = s$

$$\nabla \cdot \mathbf{J}_i = \frac{s_i}{M_i}$$

"Effective binary" or heat conduction: $\mathbf{q} = -D\nabla\phi$

Constant diffusivity: $\nabla^2 \phi = -\frac{s}{D}$

One-dimensional: $\frac{\mathrm{d}^2\phi}{\mathrm{d}z^2} = -\frac{s}{D}$



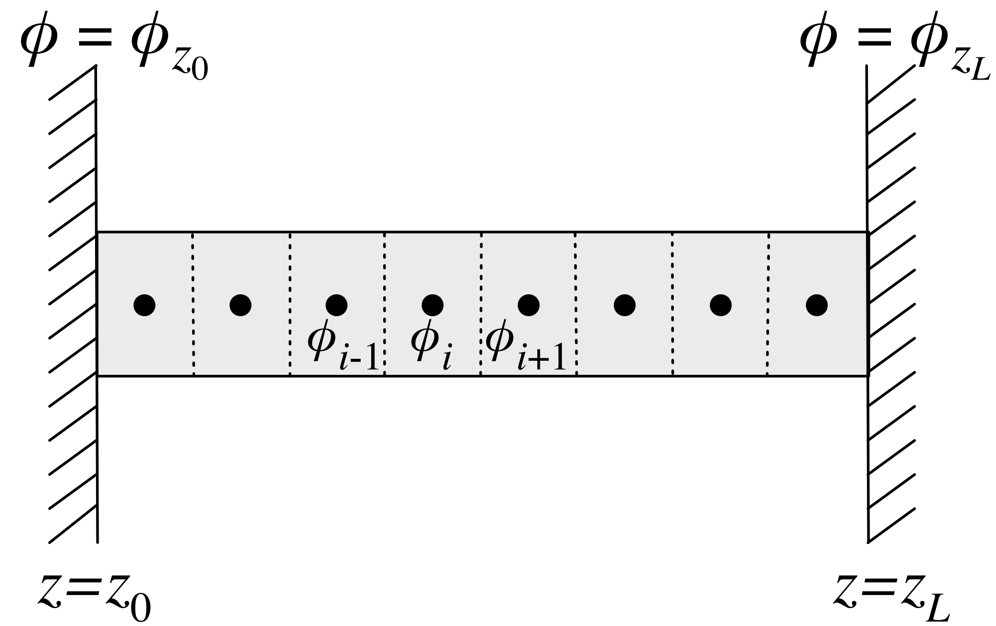

$$\left.\frac{\mathrm{d}^2\phi}{\mathrm{d}z^2}\right|_i = \frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta z^2} + \mathcal{O}(\Delta z^2)$$

$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta z^2} = -\frac{s_i}{D}$$

We can apply this at all "interior" points. At the boundaries, we must modify this....

# Dirichlet Boundary Conditions

If the solution variable is known at the boundary, then we call this a **Dirichlet** boundary condition.




$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta z^2} = -\frac{s_i}{D}$$

This applies at all interior points, $2 \le i \le n\text{-}1$.

Linear interpolation between "0" and "1"

At $z_0$, $\phi$=$\phi_{z0}$.

$$\frac{\phi_0 + \phi_1}{2} = \phi_{z_0} \;\Rightarrow\; \phi_0 = 2\phi_{z_0} - \phi$$

Using the top equation,

$$\frac{\phi_2 - 3\phi_1}{\Delta z^2} = -\frac{s_1}{D} - \frac{2\phi_{z_0}}{\Delta z^2}$$

applies at $i$=1.

At $z_L$, $\phi$=$\phi_{zL}$.

$$\frac{\phi_{n+1} + \phi_n}{2} = \phi_{z_L} \;\Rightarrow\; \phi_{n+1} = 2\phi_{z_L} - \phi_n$$

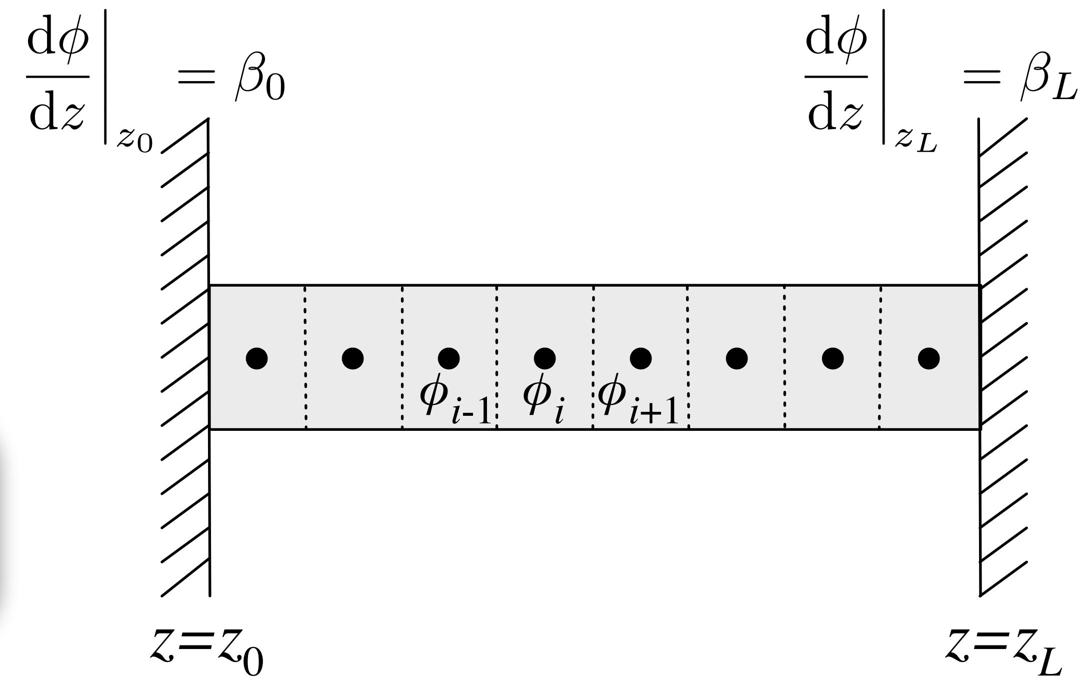
Using the top equation,

$$\frac{\phi_{n-1} - 3\phi_n}{\Delta z^2} = -\frac{s_n}{D} - \frac{2\phi_{z_L}}{\Delta z^2}$$

applies at $i$=$n$.

# Neumann Boundary Conditions

If the derivative solution variable is known at the boundary, then we call this a **Neumann** boundary condition.




$$\frac{\phi_{i+1} - 2\phi_i + \phi_{i-1}}{\Delta z^2} = -\frac{s_i}{D}$$ This applies at all interior points, $2 \le i \le n\text{-}1$.

At $i$=1, $$\frac{\phi_1 - \phi_0}{\Delta z} = \beta_0 \quad \Rightarrow \quad \phi_0 = \phi_1 - \beta_0 \Delta z$$

Using the top equation, $$\frac{-\phi_1 + \phi_2}{\Delta z^2} = -\frac{s_1}{D} - \frac{\beta_0}{\Delta z}$$ applies at $i$=1.

At $i$=$n$, $$\frac{\phi_{n+1} - \phi_n}{\Delta z} = \beta_L \quad \Rightarrow \quad \phi_{n+1} = \beta_L \Delta z + \phi_n$$

Using the top equation, $$\frac{-\phi_n + \phi_{n-1}}{\Delta z^2} = -\frac{s_n}{D} - \frac{\beta_L}{\Delta z}$$ applies at $i$=$n$.

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# Example: Steady Conduction

If it were species rather than temperature, then this looks like a "Diffusion-reaction balance"

$$\frac{\mathrm{d}^2T}{\mathrm{d}z^2} = -\frac{s(z)}{\lambda} \qquad s = \exp\left(-\frac{\left(z-\frac{L}{2}\right)^2}{\gamma}\right)$$

Boundary conditions:

$$\begin{aligned} T(z=0) &= 0 \\ \left.\frac{\mathrm{d}T}{\mathrm{d}z}\right|_{z=L} &= 0 \end{aligned}$$

$$\begin{aligned} \lambda &= 10^{-3} \\ \gamma &= 10^{-3} \\ L &= 1 \end{aligned}$$

Find $T(z)$.

**Steps**:

1. Write down the discrete equations for interior
2. Write discrete equations at the boundary.
3. Write the matrix to be solved.
4. Finally, go to Matlab to solve the problem.

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Interior equations $(1 < i < n)$

$$\frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta z^2} = -\frac{s_i}{\lambda} \qquad s_i = \exp\left(-\frac{\left(z_i - \frac{L}{2}\right)^2}{\gamma}\right)$$

Left Boundary $(i = 1)$

$$\frac{T_0 - 2T_1 + T_2}{\Delta z^2} = -\frac{s_1}{\lambda}$$

(must eliminate $T_0$)

$$\frac{T_1 + T_0}{2} = T(z=0) = 0$$

$$\frac{-3T_1 + T_2}{\Delta z^2} = -\frac{s_1}{\lambda}$$

Right Boundary $(i = n)$

$$\frac{T_{n-1} - 2T_n + T_{n+1}}{\Delta z^2} = -\frac{s_n}{\lambda}$$

(must eliminate $T_{n+1}$)

$$\frac{T_{n+1} - T_n}{\Delta z} = \left.\frac{\mathrm{d}T}{\mathrm{d}z}\right|_{z=L} = 0$$

$$\frac{T_{n-1} - T_n}{\Delta z^2} = -\frac{s_n}{\lambda}$$

For 5 control volumes, we have:

Left boundary condition

$$\begin{bmatrix} \boxed{-3 \quad 1} & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & \boxed{1 \quad -1} \end{bmatrix} \begin{pmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \\ T_5 \end{pmatrix} = -\frac{\Delta z^2}{\lambda} \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \\ s_5 \end{pmatrix}$$

Right boundary condition

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# Nonlinear BVPs

Example: $$\frac{\mathrm{d}^2 T}{\mathrm{d}x^2} = -\alpha \left(T^4 - T_\infty^4\right)$$

$$\left.\frac{\mathrm{d}^2 T}{\mathrm{d}x^2}\right|_i \approx \frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2}$$

Nonlinear term

Discrete equation to solve at each "interior" point

$$\frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2} = -\alpha \left(T_i^4 - T_\infty^4\right)$$

## Options:

1. Leave $T_i^4$ on the right hand side & try to solve the linear system (***not*** a good option).
2. Solve the nonlinear system of equations using Newton's method.
   - rewrite in residual form
   - requires a Jacobian matrix
   - This is the most general approach (big hammer)
3. *Linearize* the equation.

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# Linearization

## Example: $y = 5x^3 - 2x$

Taylor series expansion about $x_o$:

$$f(x) = f(x_o) + f'(x_0)(x - x_o) + \frac{1}{2} f''(x_o)(x - x_o)^2 + \cdots + \frac{1}{n!} f^{(n)}(x_o)(x - x_o)^{n+1}$$

$$\begin{aligned} y &\approx 5x_o^3 - 2x_o + \left(15x_o^2 - 2\right)(x - x_o) \\ &= -10x_o^3 + (15x_o^2 - 2)x \end{aligned}$$

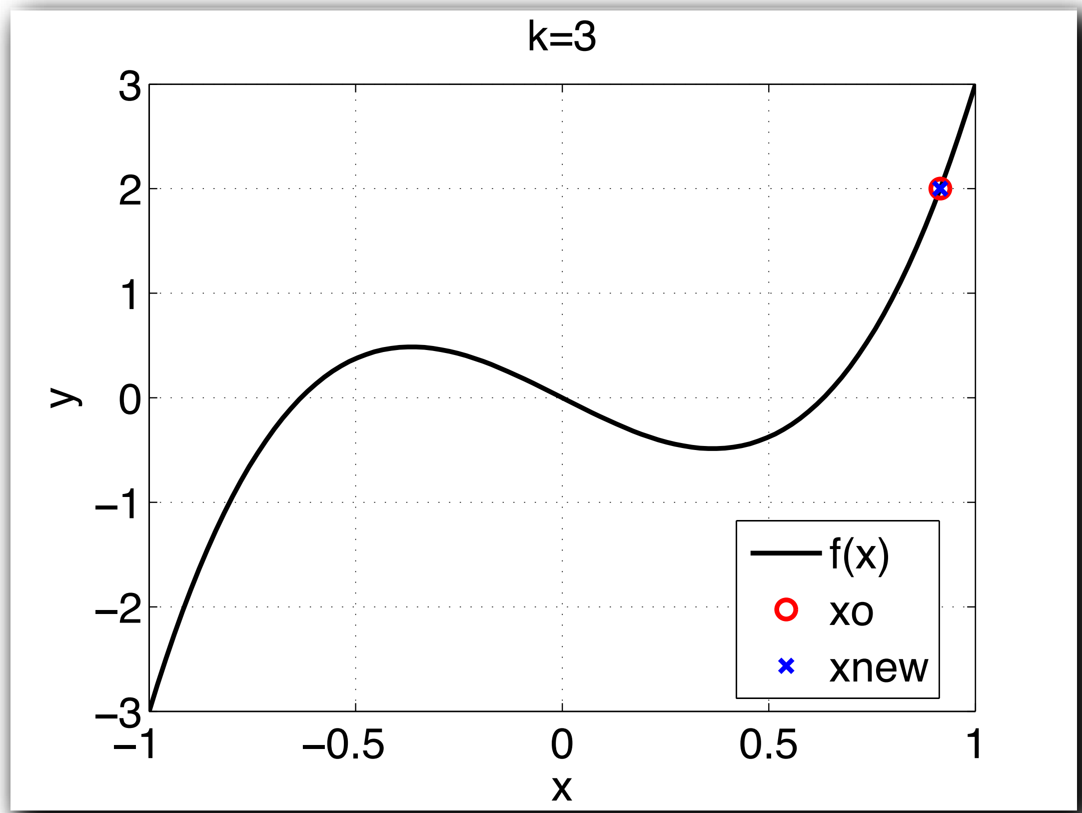
Now $y$ is *linear* with respect to $x$ (nonlinear with respect to $x_o$).

<u>Example</u>: Solve for $x$ such that $y$=2.

$$x = \frac{y + 10x_o^3}{15x_o^2 - 2}$$

1. Guess $x_o$.
2. Calculate new value for $x$.
3. if $|x - x_o| > \varepsilon$ then $x_o = x$, return to step 2. Otherwise, done!

| $k$ | $x_o$ | $x$ |
|---|---|---|
| 1 | 1 | 0.9231 |
| 2 | 0.9231 | 0.9151 |
| 3 | 0.9151 | 0.9150 |




<u>Exercise</u>: what happens when we change our initial guess to $x$=0?

# Linearization for Nonlinear BVPs

$$\frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2} = -\alpha \left( T_i^4 - T_\infty^4 \right)$$

Linearize $T_i^4$ term about $T_i^*$:

$$T_i^4 \approx (T_i^*)^4 + 4(T_i^*)^3(T_i - T_i^*)$$

$$\frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2} = -\alpha \left[ (T_i^*)^4 + 4(T_i^*)^3(T_i - T_i^*) - T_\infty^4 \right]$$

$$\frac{1}{\Delta x^2} T_{i-1} - \left( \frac{2}{\Delta x^2} + 4\alpha (T_i^*)^3 \right) T_i + \frac{1}{\Delta x^2} T_{i+1} = \alpha \left[ 3(T_i^*)^4 + T_\infty^4 \right]$$

Applies to all interior points.

$$\begin{bmatrix} BC_1 & & & \\ \frac{1}{\Delta x^2} & -\left(\frac{2}{\Delta x^2} + 4\alpha(T_2^*)^3\right) & \frac{1}{\Delta x^2} & 0 \\ \ddots & \ddots & \ddots & \\ 0 & \frac{1}{\Delta x^2} & -\left(\frac{2}{\Delta x^2} + 4\alpha(T_{n-1}^*)^3\right) & \frac{1}{\Delta x^2} \\ & & & BC_n \end{bmatrix} \begin{pmatrix} T_1 \\ T_2 \\ \vdots \\ T_{n-1} \\ T_n \end{pmatrix} = \begin{pmatrix} bc_1 \\ \alpha \left[ 3(T_2^*)^4 + T_\infty^4 \right] \\ \vdots \\ \alpha \left[ 3(T_{n-1}^*)^4 + T_\infty^4 \right] \\ bc_n \end{pmatrix}$$

Boundary conditions implemented as previously discussed.

1. Guess the solution values ($T_i^*$)
2. Update the LHS matrix and RHS vector given these values for $T_i^*$.
3. Solve the system of equations for $T_i$.
4. If $\|T_i - T_i^*\| > \varepsilon$ then set $T_i^* = T_i$ and return to step 2. Otherwise, we have the answer.

You choose the norm you want ($L_2$, $L_\infty$)

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# "Elliptic" PDEs

In chemical engineering applications, elliptic PDEs typically arise from ***steady-state*** diffusion problems.

$$\nabla^2 \phi = f(\vec{x}, \phi)$$

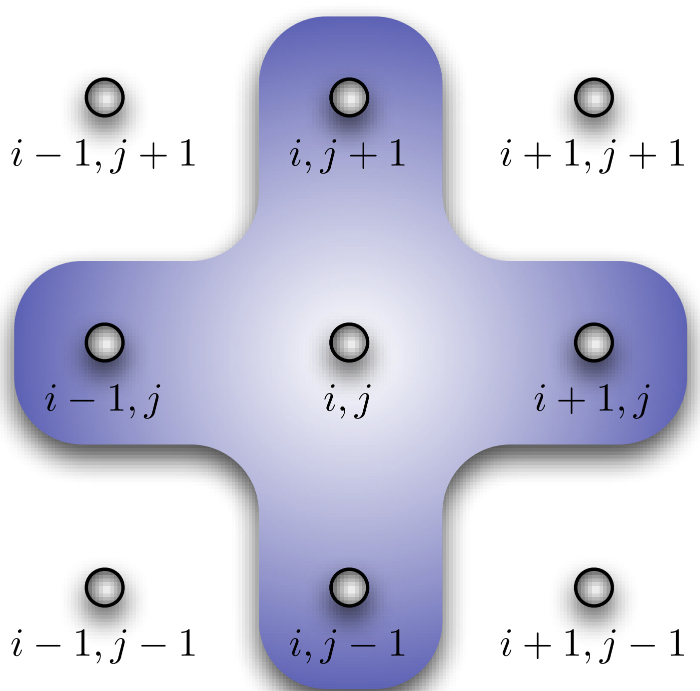
two-dimensional rectangular coordinates

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = f(x, y, \phi)$$

Second-order discretization:

$$\frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{\Delta x^2} + \frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}}{\Delta y^2} = f(x_{i,j}, y_{i,j}, \phi_{i,j})$$

Applies at all "interior" points.




- At $i$=1, and $i$=$n_x$ apply $x$ boundary conditions.
- At $j$=1, and $j$=$n_y$ apply $y$ boundary conditions.

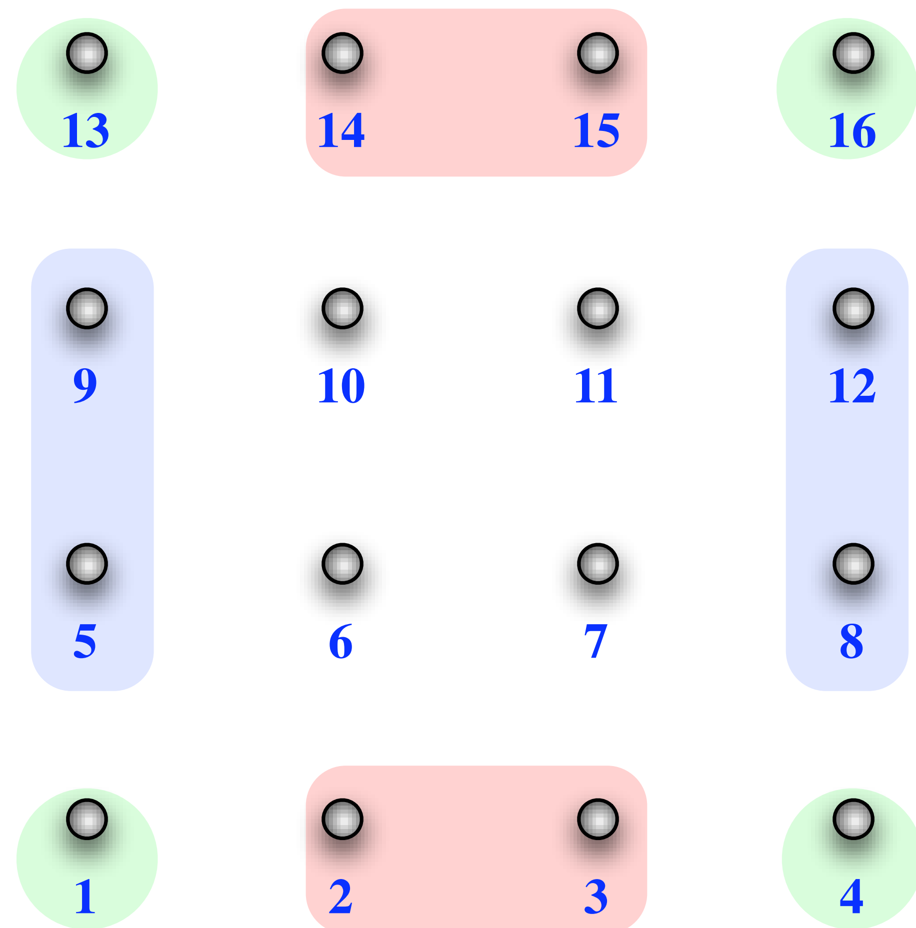
**Variable numbering (4x4 grid)**

- (x,y) layout
- solution index (eqn #) layout

| | | | |
|---|---|---|---|
| 1,4<br>13 | 2,4<br>14 | 3,4<br>15 | 4,4<br>16 |
| 1,3<br>9 | 2,3<br>10 | 3,3<br>11 | 4,3<br>12 |
| 1,2<br>5 | 2,2<br>6 | 3,2<br>7 | 4,2<br>8 |
| 1,1<br>1 | 2,1<br>2 | 3,1<br>3 | 4,1<br>4 |

$$\frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{\Delta x^2} + \frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}}{\Delta y^2} = f(x_{i,j}, y_{i,j}, \phi_{i,j})$$

<u>Note</u>: if $f(x,y)$ depends on $\boldsymbol{\phi}$ then this is a system of ***nonlinear*** equations!




$$\left[\begin{array}{cccccccccccccccc}
BC & ?? & 0 & 0 & ?? & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2} & \frac{1}{\Delta x^2} & 0 & 0 & ?? & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\Delta x^2} & -\frac{2}{\Delta x^2} & \frac{1}{\Delta x^2} & 0 & 0 & ?? & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & ?? & BC & 0 & 0 & 0 & ?? & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{\Delta y^2} & 0 & 0 & 0 & -\frac{2}{\Delta x^2} & ?? & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \frac{1}{\Delta y^2} & 0 & 0 & \frac{1}{\Delta x^2} & -2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) & \frac{1}{\Delta x^2} & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & \frac{1}{\Delta x^2} & -2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) & \frac{1}{\Delta x^2} & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & ?? & -\frac{2}{\Delta y^2} & 0 & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & 0 & -\frac{2}{\Delta y^2} & ?? & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & \frac{1}{\Delta x^2} & -2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) & \frac{1}{\Delta x^2} & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & \frac{1}{\Delta x^2} & -2\left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}\right) & \frac{1}{\Delta x^2} & 0 & 0 & \frac{1}{\Delta y^2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\Delta y^2} & 0 & 0 & ?? & -\frac{2}{\Delta y^2} & 0 & 0 & 0 & \frac{1}{\Delta y^2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & ?? & 0 & 0 & 0 & BC & ?? & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & ?? & 0 & 0 & \frac{1}{\Delta x^2} & \frac{-2}{\Delta x^2} & \frac{1}{\Delta x^2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & ?? & 0 & 0 & \frac{1}{\Delta x^2} & \frac{-2}{\Delta x^2} & \frac{1}{\Delta x^2} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & ?? & 0 & 0 & ?? & BC
\end{array}\right]
\begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \\ \phi_5 \\ \phi_6 \\ \phi_7 \\ \phi_8 \\ \phi_9 \\ \phi_{10} \\ \phi_{11} \\ \phi_{12} \\ \phi_{13} \\ \phi_{14} \\ \phi_{15} \\ \phi_{16} \end{pmatrix}
=
\begin{pmatrix} bc_1 \\ f(x_2,y_2,\phi_2) + bc_2 \\ f(x_3,y_3,\phi_3) + bc_3 \\ bc_4 \\ f(x_5,y_5,\phi_5) + bc_5 \\ f(x_6,y_6,\phi_6) \\ f(x_7,y_7,\phi_7) \\ f(x_8,y_8,\phi_8) + bc_8 \\ f(x_9,y_9,\phi_9) + bc_9 \\ f(x_{10},y_{10},\phi_{10}) \\ f(x_{11},y_{11},\phi_{11}) \\ f(x_{12},y_{12},\phi_{12}) + bc_{12} \\ f(x_7,y_7,\phi_7) + bc_{13} \\ f(x_{14},y_{14},\phi_{14}) + bc_{14} \\ f(x_{15},y_{15},\phi_{15}) + bc_{15} \\ bc_{16} \end{pmatrix}$$

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# Parabolic PDEs

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \frac{\partial^2 T}{\partial x^2} + s_T$$

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# Ordinary Differential Equations (ODEs)

A coupled system of ODEs: $$\frac{\mathrm{d}\phi_i}{\mathrm{d}t} = F_i(\phi_j)$$

**Explicit:**

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = F_i(\phi_j^n) + \mathcal{O}(\Delta t)$$

**Use for:**
- "Non-stiff" equations
- Unsteady solutions

**Implicit:**

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = F_i(\phi_j^{n+1}) + \mathcal{O}(\Delta t)$$

$$\Downarrow$$

$$r_i = F_i(\phi_j^{n+1}) - \frac{\phi^{n+1} - \phi^n}{\Delta t}$$

System of nonlinear equations. Solve for $r_i = 0$.

**Use for:**
- "Stiff" equations
- Time-marching to steady solutions

Higher-order methods can be constructed. (Runge Kutta, *etc.*)

MATLAB: **`ode45`** (nonstiff), **`ode23s`** (stiff)

You provide evaluation of $F_i(\phi_j)$

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# Example: Kinetics

$$A + B \xrightarrow{k_1} C$$
$$A + C \xrightarrow{k_2} D$$

$$\begin{aligned}
\frac{\mathrm{d}C_A}{\mathrm{d}t} &= -r_1 - r_2 \\
\frac{\mathrm{d}C_B}{\mathrm{d}t} &= -r_1 \\
\frac{\mathrm{d}C_C}{\mathrm{d}t} &= r_1 - r_2 \\
\frac{\mathrm{d}C_D}{\mathrm{d}t} &= r_2
\end{aligned}$$

Initial conditions: $C_A=1, C_B=0.6.$

Rate constants: $k_1=1, k_2=0.1.$

- Plot concentrations as functions of time.
  - requires solution of system of ODEs
- Determine the equilibrium composition.
  - Use stoichiometry & mole balance
- How long to achieve 99% of equilibrium?
  - find this entry in the ODE solution history.

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# "Parabolic" PDEs

Parabolic PDEs are characterized primarily by ***transient diffusion***.

Transient diffusion equation
(constant diffusivity, $\Gamma$)

$$\frac{\partial \phi}{\partial t} = \Gamma \nabla^2 \phi + s_\phi$$

Transient temperature diffusion equation
(constant pressure, diffusivity)

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \nabla^2 T + s_T$$

Transient temperature diffusion equation
(two-dimensional version of the above equation)

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + s_T$$

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# Solving Time-Dependent PDEs

## The "Method of Lines"

$$\frac{\partial \phi}{\partial t} = \Gamma \frac{\partial^2 \phi}{\partial x^2} + s$$

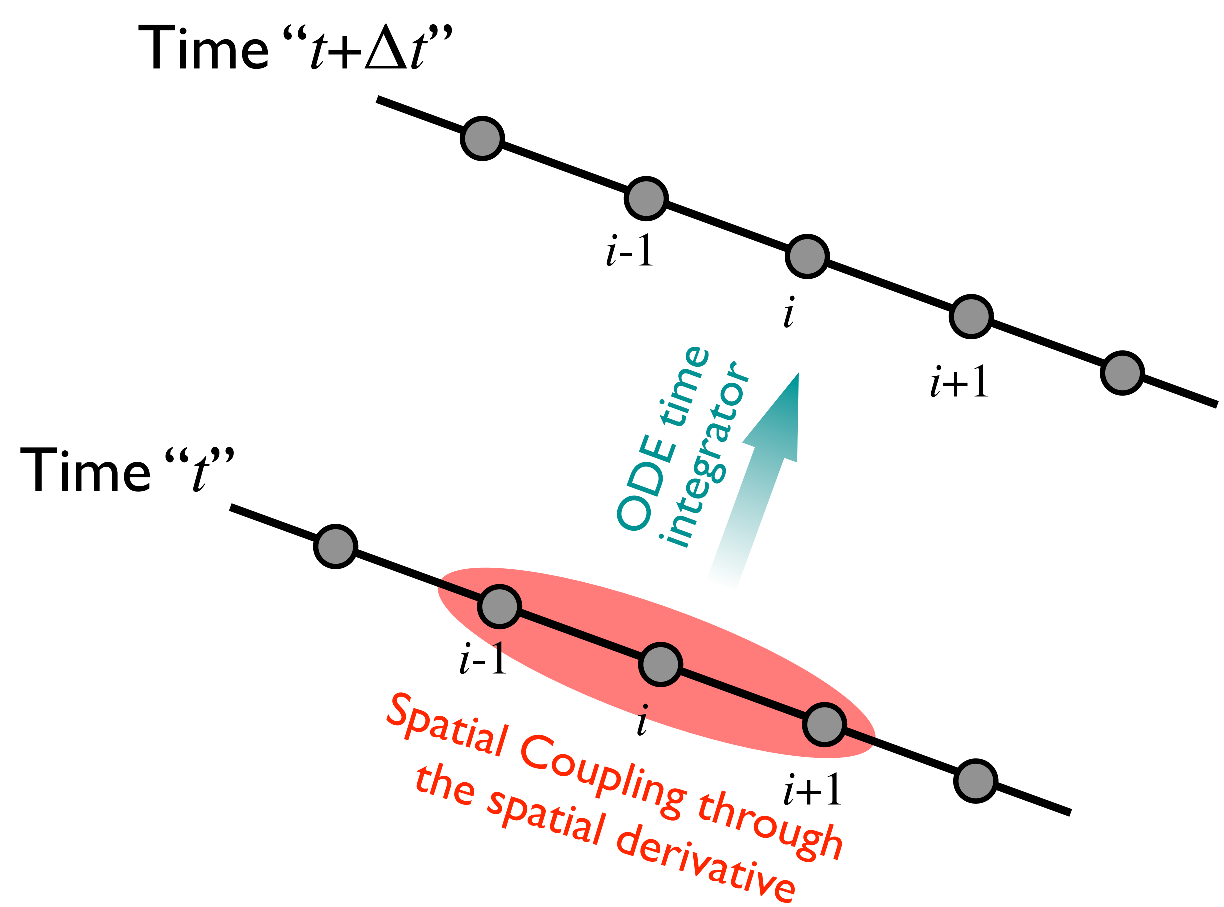
Spatial discretization:

$$\frac{\partial^2 \phi}{\partial x^2} \approx \frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2}$$

$$\frac{\partial \phi_i}{\partial t} = \Gamma_i \frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2} + s_i$$

This is a *system* of coupled ODEs.

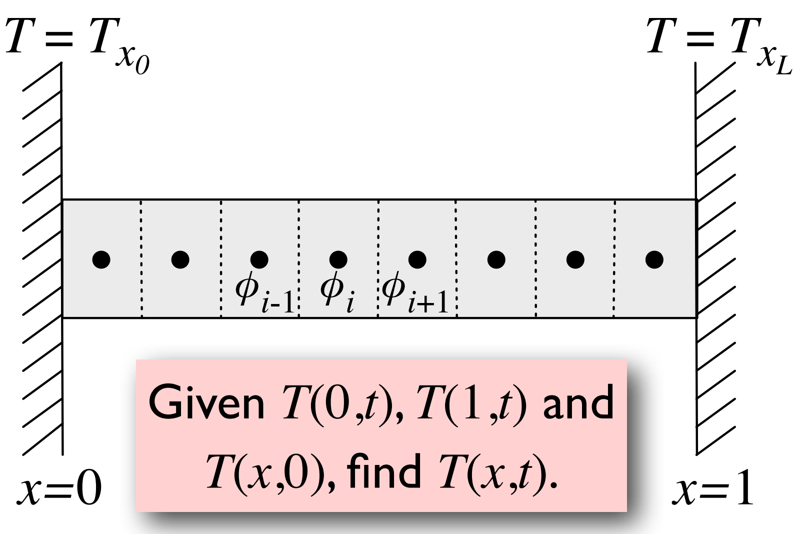
$$\begin{aligned}
\frac{\partial \phi_1}{\partial t} &= ? \text{ Need to use BC information...} \\
\frac{\partial \phi_2}{\partial t} &= \Gamma \frac{\phi_1 - 2\phi_2 + \phi_3}{\Delta x^2} + s_2, \\
\vdots &= \vdots \\
\frac{\partial \phi_{n-1}}{\partial t} &= \Gamma \frac{\phi_{n-2} - 2\phi_{n-1} + \phi_n}{\Delta x^2} + s_{n-1}, \\
\frac{\partial \phi_n}{\partial t} &= ? \text{ Need to use BC information...}
\end{aligned}$$




Solve using Matlab's **`ode45`** or **`ode23s`**.

# Example 1

## (Dirichlet Boundary Conditions)




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

$$\begin{aligned} T(0,t) &= 0, && \text{BC at } x=0 \\ T(1,t) &= 0, && \text{BC at } x=1 \\ T(x,0) &= \phi(x) && \text{Initial condition} \end{aligned}$$

**Analytical solution:**

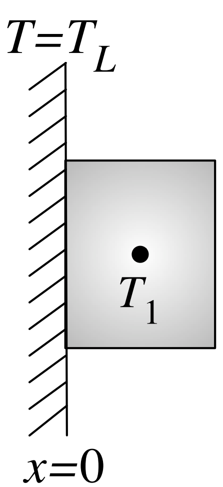
$$T(x,t) = \sum_{k=1}^{\infty} A_k e^{-k^2\pi^2\alpha t} \sin(k\pi x) \qquad A_k = 2\int_0^1 \phi(x)\sin(k\pi x)\mathrm{d}x$$

**Numerical solution:**

$$\frac{\partial T_i}{\partial t} = \alpha \frac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2}$$

Applies at all "interior" points ($i$=2, ... ,$n$-1)

What do we do at the boundaries ($i$=1, $i$=$n$)?




$$\frac{\partial T_1}{\partial t} = \alpha \frac{T_0 - 2T_1 + T_2}{\Delta x^2} \qquad T_{x_0} = \frac{T_1 + T_0}{2} \Rightarrow T_0 = 2T_{x_0} - T_1 \qquad \frac{\partial T_1}{\partial t} = \alpha \frac{2T_{x_0} - 3T_1 + T_2}{\Delta x^2}$$

A similar procedure at $x$=$L$ leads to:

$$\frac{\partial T_n}{\partial t} = \alpha \frac{2T_{x_L} - 3T_n + T_{n-1}}{\Delta x^2}$$

Solve this problem for $t$ = [ 0, 240 ] seconds given:

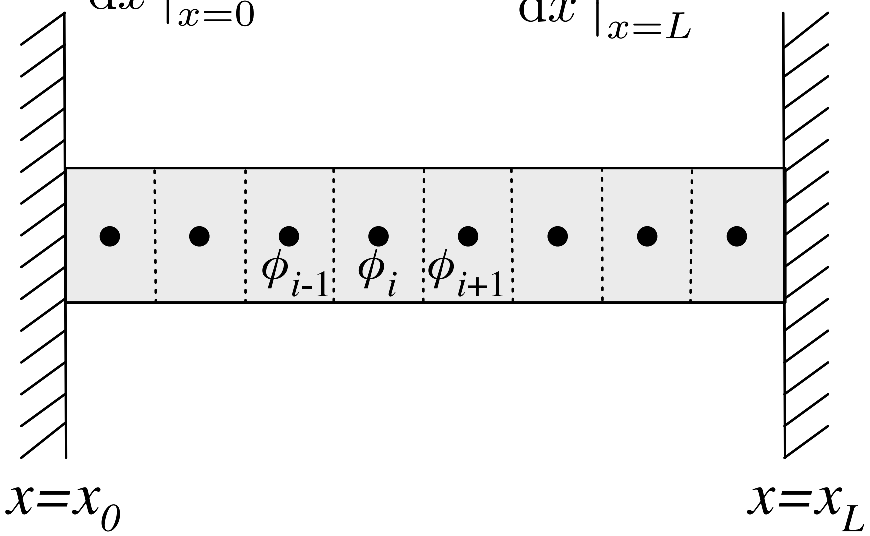
$$\phi(x) = \exp\left(-100(x-0.3)^2\right)$$

$$\alpha = \frac{\lambda}{\rho c_p} = 10^{-}4 \ \frac{\mathrm{m}^2}{\mathrm{s}}$$

# Example 2

## (Neumann Boundary Conditions)

$$\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{x=0} = \beta_0 \qquad \left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{x=L} = \beta_L$$

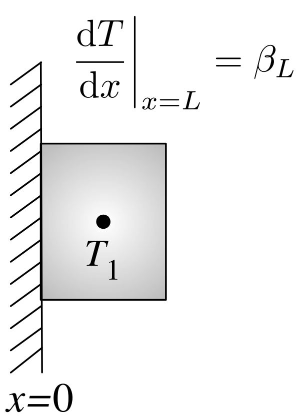



$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

$$\begin{aligned} \left.\frac{\partial T}{\partial x}\right|_{0,t} &= \beta_0, && \text{BC at } x\text{=0} \\ \left.\frac{\partial T}{\partial x}\right|_{1,t} &= \beta_L, && \text{BC at } x\text{=1} \\ T(x,0) &= \phi(x) && \text{Initial condition} \end{aligned}$$

Numerical solution: $\dfrac{\partial T_i}{\partial t} = \alpha \dfrac{T_{i-1} - 2T_i + T_{i+1}}{\Delta x^2}$ Applies at all "interior" points ($i$=2 ... $n$-1)

What do we do at the boundaries ($i$=1, $i$=$n$)?




$$\frac{\partial T_1}{\partial t} = \alpha \frac{T_0 - 2T_1 + T_2}{\Delta x^2}$$

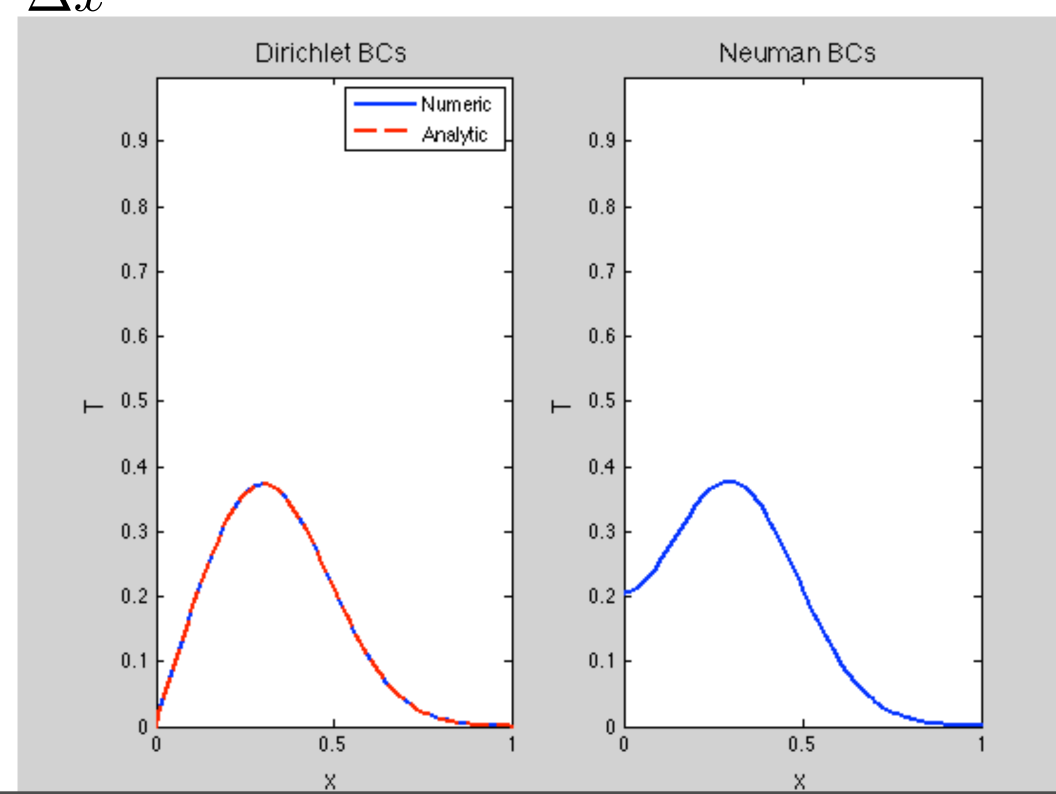
Need to eliminate $T_0$.

$$\left.\frac{\mathrm{d}T}{\mathrm{d}x}\right|_{x=0} = \frac{T_1 - T_0}{\Delta x} = \beta_0 \quad \Rightarrow \quad T_0 = T_1 - \beta_0 \Delta x$$

$$\frac{\partial T_1}{\partial t} = \alpha \left( \frac{T_2 - T_1}{\Delta x^2} - \frac{\beta_0}{\Delta x} \right) \quad \text{at } i\text{=1.}$$

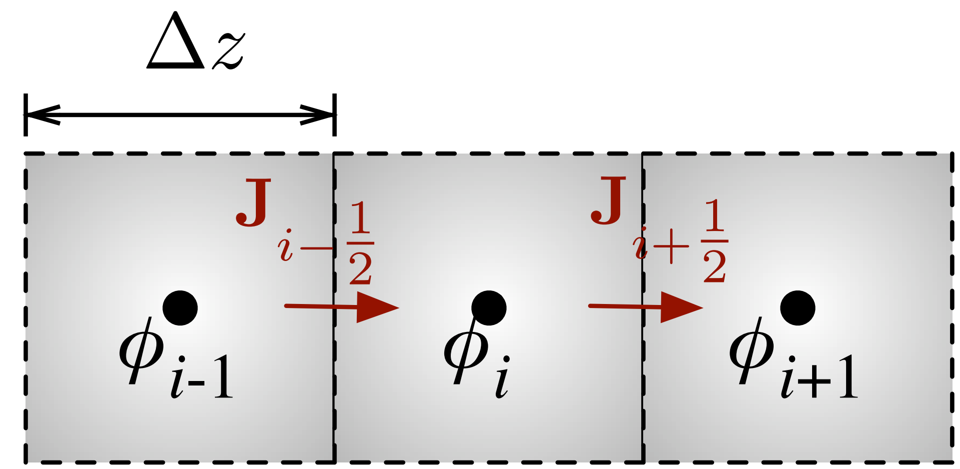
Using the same analysis at $x$=1 ($i$=$n$)...

$$\frac{\partial T_n}{\partial t} = \alpha \frac{T_{n-1} - T_n}{\Delta x^2} + \frac{\alpha}{\Delta x}\beta_L \quad \text{at } i\text{=}n.$$




Solve this problem given $\beta_0$=$\beta_L$=0 and the same conditions as on the previous slide.

# General Fluxes




$$\frac{\partial (x)}{\partial t} = -\frac{1}{c_t}\frac{\partial (\mathbf{J})}{\partial z} \qquad (\mathbf{J}) = -c_t [D] \left( \frac{\partial x}{\partial z} \right)$$

What have we assumed here?

$$\frac{\partial (x)_i}{\partial t} = -\frac{1}{c_t} \frac{(\mathbf{J})_{i+\frac{1}{2}} - (\mathbf{J})_{i-\frac{1}{2}}}{\Delta z}$$

Applies at $i$=1…$n$.

NOTE: "$i$" denotes a spatial index, not a species index.

$$(\mathbf{J})_{i-\frac{1}{2}} = -c_t [D]_{i-\frac{1}{2}} \frac{(x)_i - (x)_{i-1}}{\Delta z}$$

At $i$=1 we need to apply BCs

$$(\mathbf{J})_{i+\frac{1}{2}} = -c_t [D]_{i+\frac{1}{2}} \frac{(x)_{i+1} - (x)_i}{\Delta z}$$

At $i$=$n$ we need to apply BCs

$n_{species}$-1 Dimensional:

$(x)$ - species mole fractions

$(\mathbf{J})$ - species diffusive fluxes

$[D]$ - Fickian diffusion coefficient matrix

# Example: Variable Effective Diffusivity

This represents $n_s$-1 coupled PDEs for the mole fractions, $x_i$.

$$\begin{aligned}\frac{\partial x_i}{\partial t} &= -\frac{1}{c_t}\nabla\cdot\mathbf{J}_i \\ &= \nabla\cdot\left(D_{i,eff}\nabla x_i\right)\end{aligned}$$

What are the assumptions?

Assume Neumann BCs: $\frac{\partial x_i}{\partial z} = 0$ @ $z$=0 and $z$=$L$

Given $Đ_{ij}$, $x_i(t=0)$, how would you solve this?

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