UNSW AUSTRALIA

Physics 3112: Experimental & Computational Physics

T1 2025

Never Stand Still | Science | School of Physics

Computational Physics: Simulation & Modeling

LECTURER (Weeks 5-9)

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Objective (Weeks 5-9)

- Solving differential equations numerically
- Eigenvalue problems in physics
- Numerical linear algebra and solving large scale problems
- Monte Carlo simulations

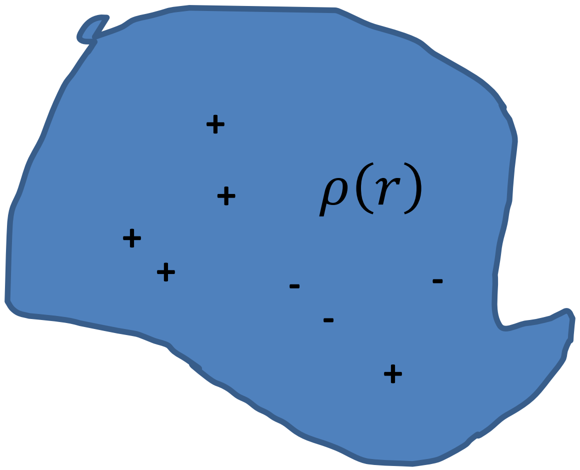
Differential Equations in Physics

Electrostatics: Poisson's Equation (Charge to Potential)

$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

$V(r), \rho(r), \qquad r = x, y, z$

$V(r)$



$$\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2}$$ (Laplacian)

Laplace Equation

$$\nabla^2 V = 0$$

Differential Equations in Physics

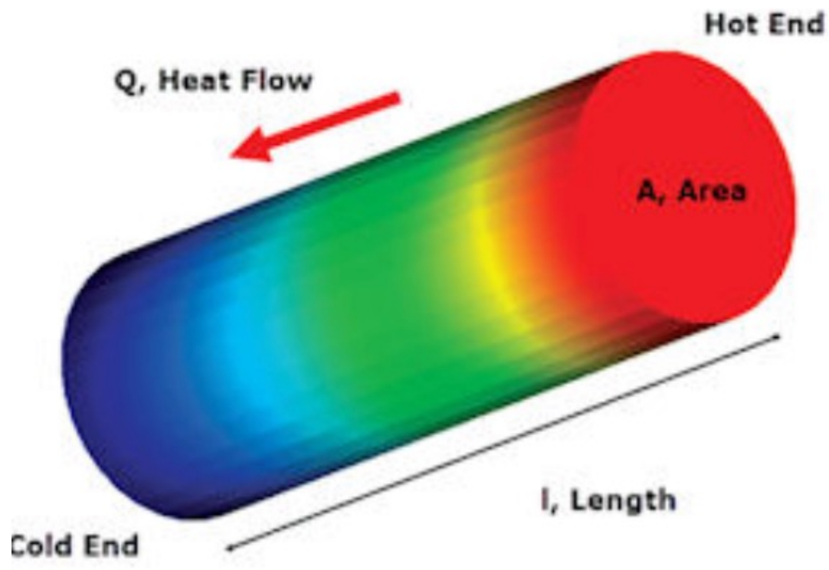
Thermal Physics: Heat Equation (2D)

$$\frac{\partial T}{\partial t}=\alpha\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)+q$$

T: Temperature

q: Heat generation rate

α: Thermal Expansion Coefficient



https://www.digitalengineering247.com/article/use-fea-thermal-analysis/

Statistical Mechanics: Motion of charge carriers

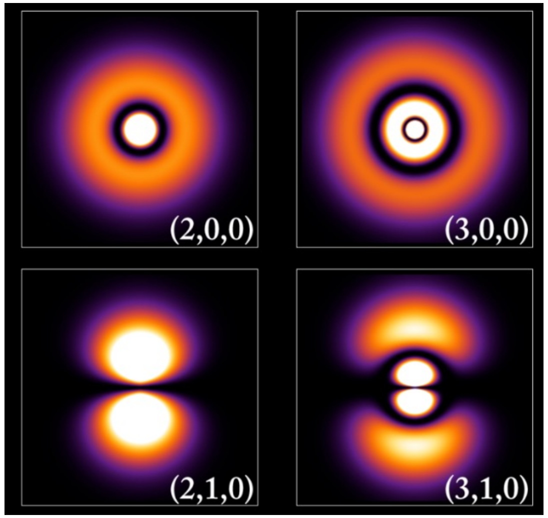
Quantum Mechanics: Time independent Schrodinger Equation (Wavefunction)

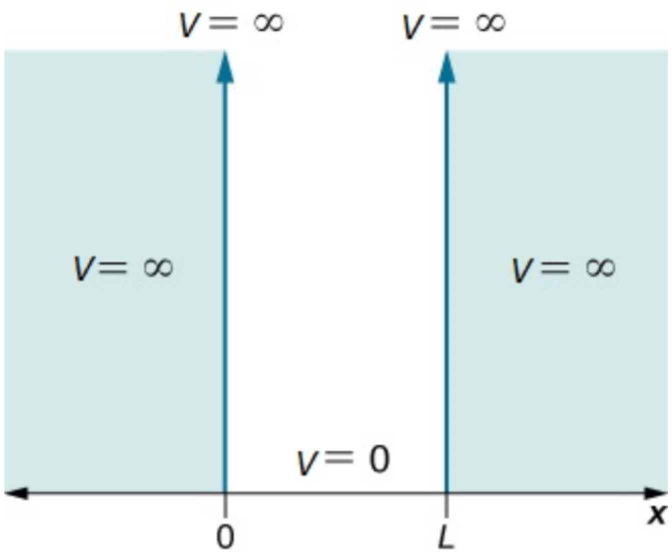
$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

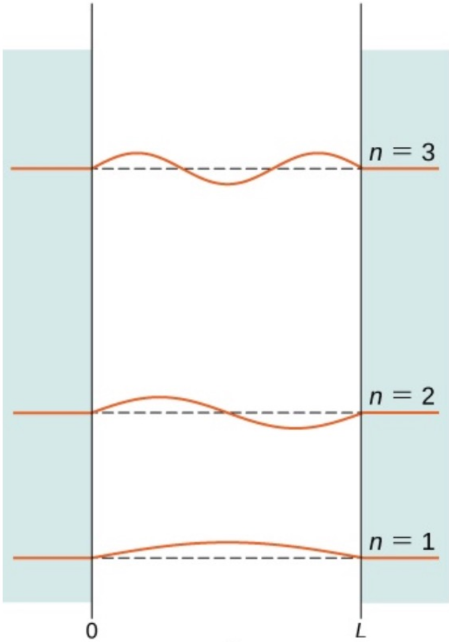
$$V(r), \psi(r), \qquad r = x, y, z$$

Particle in a box wavefunction

Atoms: Solution with 1/r potential







https://en.wikipedia.org/wiki/Atomic_orbital#/media/File:Hydrogen_Density_Plots.png

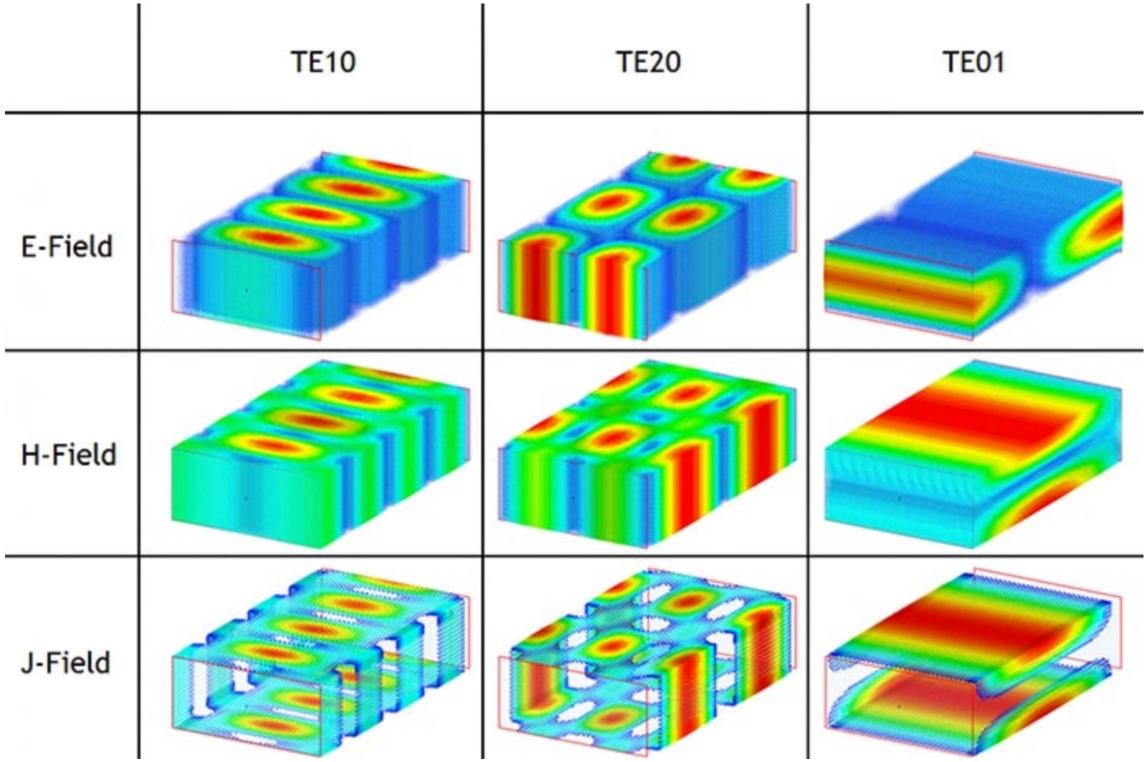
https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Map%3A_Physical_Chemistry_(McQuarrie_and_Simon)/03%3A_The_Schr%C3%B6dinger_Equation_and_a_Particle_in_a_Box/3.05%3A_The_Energy_of_a_Particle_in_a_Box_is_Quantized

Electro-magnetics: Maxwell's Equation (Electric & Magnetic Fields)

Wave Guides

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$



https://www.technobyte.org/wp-content/uploads/2016/11/Rect-Hollow-WG-Modes.jpg

Differential Equations in Physics

Electrostatics: Poisson's Equation (Charge to Potential)

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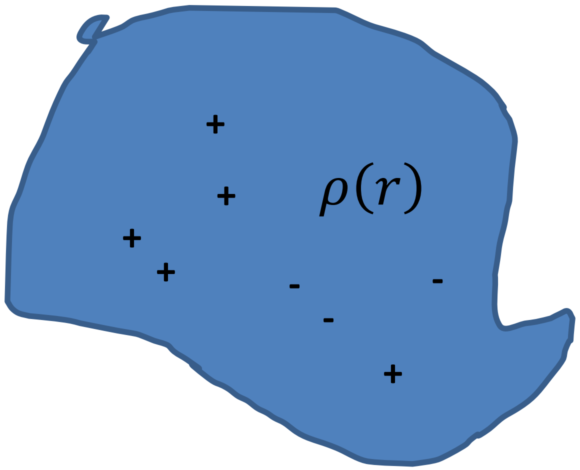
$$V(r), \rho(r), \qquad r = x, y, z$$

$V(r)$

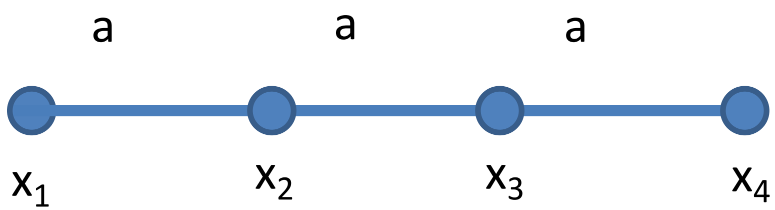


$$\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \qquad \text{(Laplacian)}$$

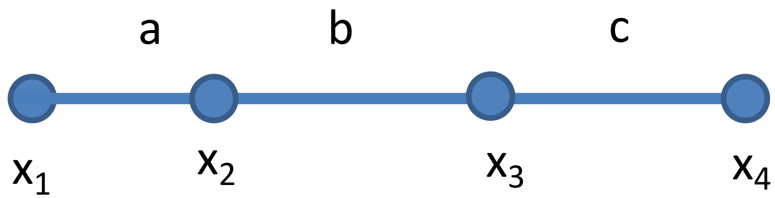
Numerical Solution of Differential Equations: The Finite Difference Method

Example: 1D Poisson's Equation with FDM $\nabla^2 V = -\frac{\rho}{\epsilon}$

Step 1: Mesh



Homogeneous mesh: Equal grid spacing



Inhomogeneous mesh: Unequal grid spacing

Needed for systems – when charge is very dense at one point and coarse in another.

Numerical Solution of Differential Equations: The Finite Difference Method

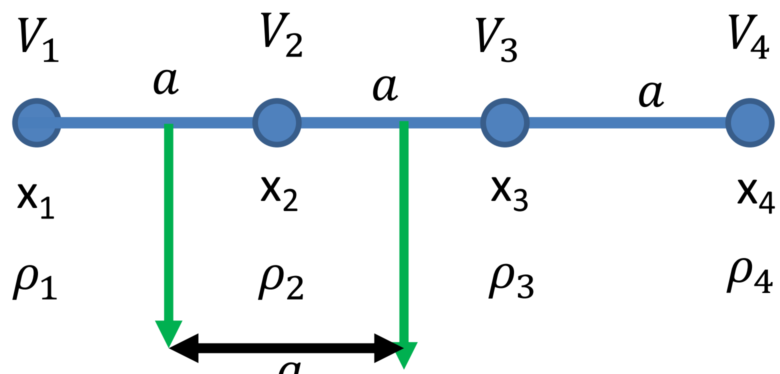
Example: 1D Poisson's Equation with FDM

$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

Output: Potential V

Step 2: Define operators

& Input / Output Variables



Input: Charge density

(Charge per unit length in 1D)

$$\nabla V = \frac{\Delta V}{\Delta x} = \qquad \frac{V_2 - V_1}{x_2 - x_1} \qquad \frac{V_3 - V_2}{x_3 - x_2}$$

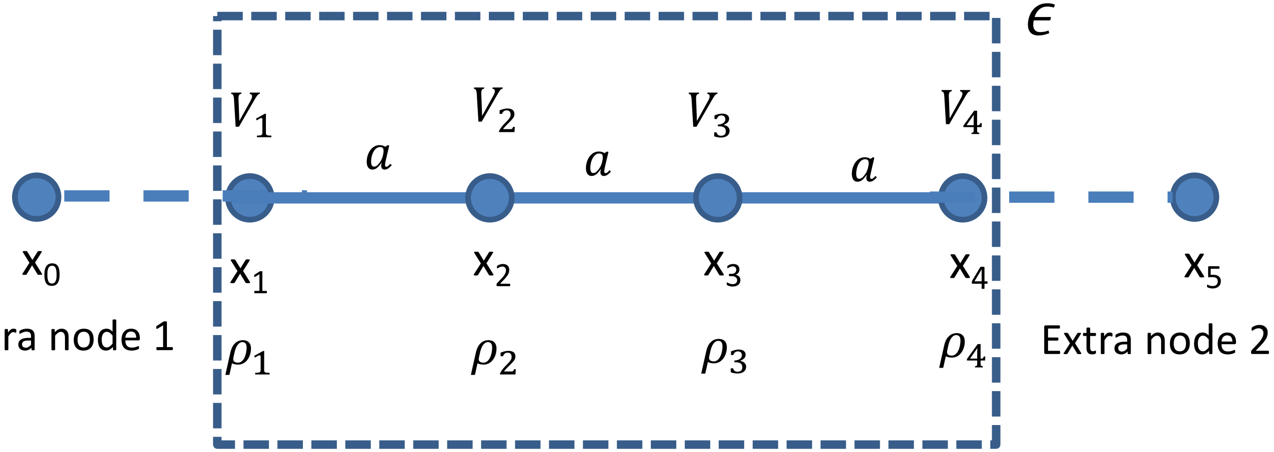
$$\frac{V_2 - V_1}{a} \qquad \frac{V_3 - V_2}{a}$$

$$\nabla^2 = \frac{d^2}{dx^2} \quad \text{(at } x_2\text{)} \qquad \frac{\frac{V_3 - V_2}{a} - \frac{V_2 - V_1}{a}}{a} \qquad \frac{V_3 - 2V_2 + V_1}{a^2}$$

Numerical Solution of Differential Equations: The Finite Difference Method

Example: 1D Poisson's Equation with FDM $\nabla^2 V = -\dfrac{\rho}{\epsilon}$

Step 3: Difference Equations



Attach two extra nodes (Boundary conditions)

$$\nabla^2 = \frac{d^2}{dx^2} = \frac{V_3 - 2V_2 + V_1}{a^2}$$

x_1	$V_2 - 2V_1 + \overset{0}{V_0} = -\rho_1 a^2/\epsilon$
x_2	$V_3 - 2V_2 + V_1 = -\rho_2 a^2/\epsilon$
x_3	$V_4 - 2V_3 + V_2 = -\rho_3 a^2/\epsilon$
x_4	$\overset{0}{V_5} - 2V_4 + V_3 = -\rho_4 a^2/\epsilon$

Boundary Conditions

V=0 at the edges

Example: 1D Poisson's Equation with FDM

x_1 $\quad V_2 - 2V_1 + \cancelto{0}{V_0} = -\rho_1 a^2/\epsilon$

x_2 $\quad V_3 - 2V_2 + V_1 = -\rho_2 a^2/\epsilon$

x_3 $\quad V_4 - 2V_3 + V_2 = -\rho_3 a^2/\epsilon$

x_4 $\quad \cancelto{0}{V_5} - 2V_4 + V_3 = -\rho_4 a^2/\epsilon$

Boundary Conditions

V=0 at the edges

Step 4: Matrix Representation

- Tri-diagonal matrix: 3 diagonals, main + 2 off-diag.
- Applies to 1D case

$$\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{bmatrix} = -\frac{a^2}{\epsilon} \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_4 \end{bmatrix}$$

$$AX = B$$

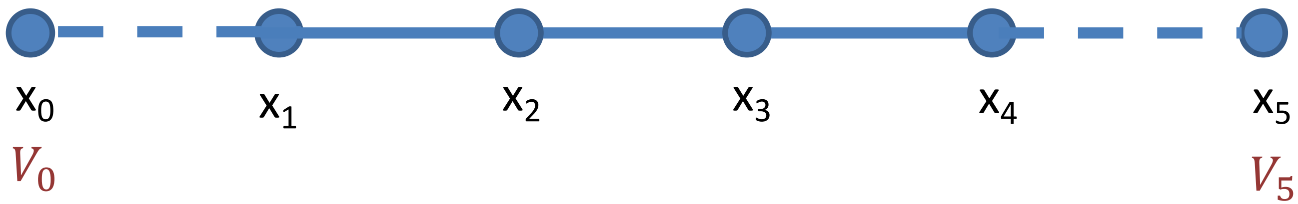
Linear (Matrix) Equation

Solve for X (V in our case)

Numerical Solution of Differential Equations: The Finite Difference Method

$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

Step 5: Boundary conditions (2 common types)



1. Dirichlet Boundary condition (BC): Set Potential/Voltage to constant values at the edges.

x_1 $\quad V_2 - 2V_1 + V_0 = -\rho_1 a^2/\epsilon \qquad V_2 - 2V_1 = -\rho_1 a^2/\epsilon - V_0$

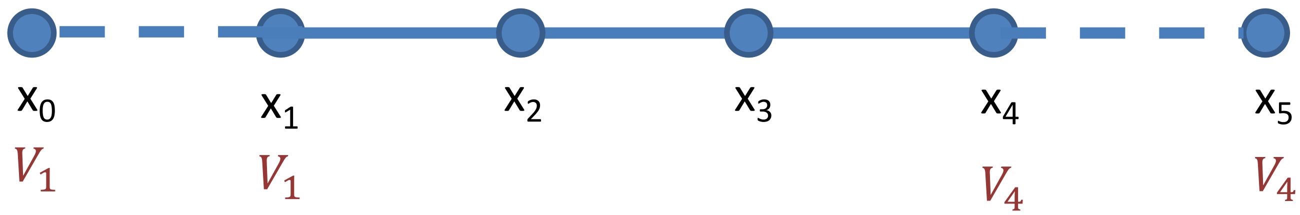
x_4 $\quad V_5 - 2V_4 + V_3 = -\rho_4 a^2/\epsilon \qquad -2V_4 + V_3 = -\rho_4 a^2/\epsilon - V_5$

$$\begin{bmatrix} -2 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{bmatrix} = -\frac{a^2}{\epsilon} \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_4 \end{bmatrix} - \begin{bmatrix} V_0 \\ 0 \\ 0 \\ V_5 \end{bmatrix}$$

Numerical Solution of Differential Equations: The Finite Difference Method

$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

Step 5: Boundary conditions (2 common types)



2. Neumann Boundary condition (BC): Set gradient of potential to constant at the edges.

$E = -\nabla V$ Constant Example: Set E=0 at the edges

x_1 $\quad V_2 - 2V_1 + V_1 = -\rho_2 a^2/\epsilon \qquad V_2 - V_1 = -\rho_1 a^2/\epsilon$

x_4 $\quad V_4 - 2V_4 + V_3 = -\rho_4 a^2/\epsilon \qquad -V_4 + V_3 = -\rho_4 a^2/\epsilon$

$$\begin{bmatrix} -1 & 1 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \end{bmatrix} = -\frac{a^2}{\epsilon} \begin{bmatrix} \rho_1 \\ \rho_2 \\ \rho_3 \\ \rho_4 \end{bmatrix}$$

The Finite Difference Method: Error & Convergence

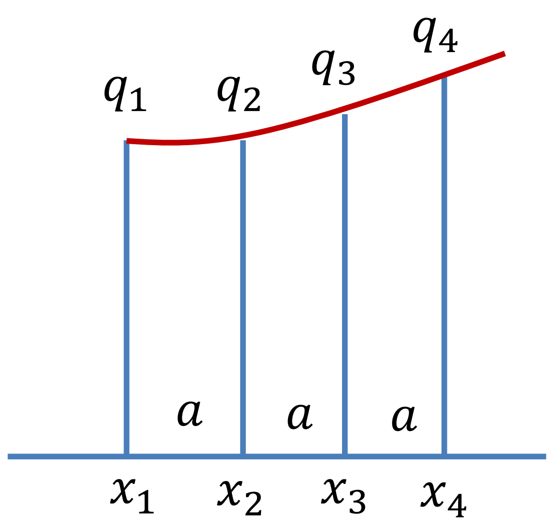
- Numerical solution is approximate.
- It approaches the exact solution in the limit grid spacing ‘a’ $\rightarrow 0$.
- Analytically unsolvable problems can be solved.

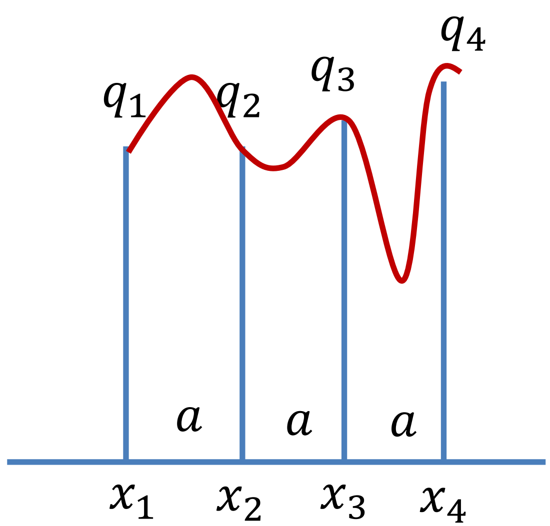
Numerical tolerance of solution

- How does the solution depend on the domain size (finite-size effects)?
- How does the solution depend on the grid spacing (meshing)?
- Order of accuracy in the definition of operators?
- Choice between accuracy and computational resources (memory and speed)?

- Define an acceptable tolerance level.
- Test the effect of various numerical parameters.
- Design simple cases to test against closed form analytic solutions.
- Build up confidence in your numerical solver.

Mesh related errors





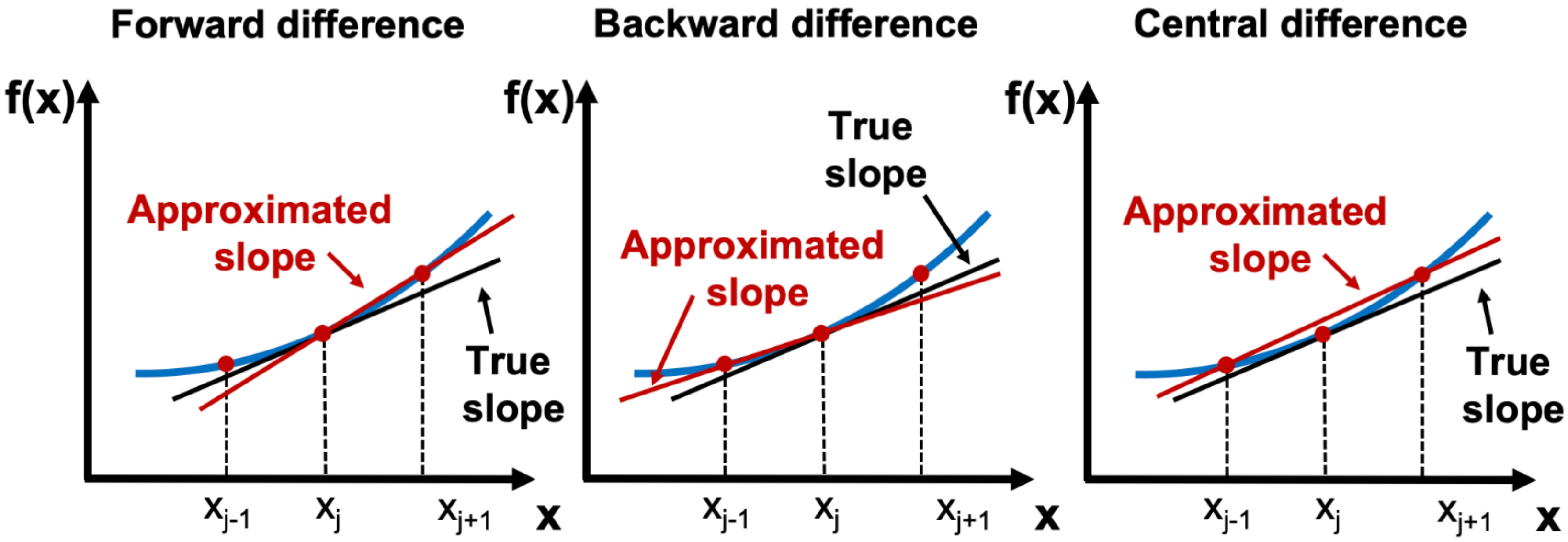
Numerical solution is good in this case.

- Curve is smooth between grid points.
- Approximately linear between grid points.

Not a good solution.

- Large variation on the scale of 'a'.
- Solution: Decrease 'a', Adaptive meshing.

Definition of operators



$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{x_{j+1} - x_j} \qquad f'(x_j) = \frac{f(x_j) - f(x_{j-1})}{x_j - x_{j-1}} \qquad f'(x_j) = \frac{f(x_{j+1}) - f(x_{j-1})}{x_{j+1} - x_{j-1}}$$

Source: https://pythonnumericalmethods.berkeley.edu/

Errors in approximating the first derivative (example)

Taylor series expansion of a function about x_j

$$f(x) = \frac{f(x_j)(x-x_j)^0}{0!} + \frac{f'(x_j)(x-x_j)^1}{1!} + \frac{f''(x_j)(x-x_j)^2}{2!} + \frac{f'''(x_j)(x-x_j)^3}{3!} + \cdots$$

Compute the derivative by forward difference (i.e. between x_j and x_{j+1}

$$f(x_{j+1}) = \frac{f(x_j)(x_{j+1} - x_j)^0}{0!} + \frac{f'(x_j)(x_{j+1} - x_j)^1}{1!} + \frac{f''(x_j)(x_{j+1} - x_j)^2}{2!} + \frac{f'''(x_j)(x_{j+1} - x_j)^3}{3!} + \cdots.$$

Grid spacing $h = x_{j+1} - x_j$

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h} + \left(-\frac{f''(x_j)h}{2!} - \frac{f'''(x_j)h^2}{3!} - \cdots\right).$$

$$f'(x_j) = \frac{f(x_{j+1}) - f(x_j)}{h} + O(h).$$

$O(h^p)$ p is the order of accuracy of the approximation

What is the order of accuracy of the central difference?

$$f(x) = \frac{f(x_j)(x-x_j)^0}{0!} + \frac{f'(x_j)(x-x_j)^1}{1!} + \frac{f''(x_j)(x-x_j)^2}{2!} + \frac{f'''(x_j)(x-x_j)^3}{3!} + \cdots$$

$$f(x_{j+1}) = f(x_j) + f'(x_j)h + \frac{1}{2}f''(x_j)h^2 + \frac{1}{6}f'''(x_j)h^3 + \cdots$$

$$f(x_{j-1}) = f(x_j) - f'(x_j)h + \frac{1}{2}f''(x_j)h^2 - \frac{1}{6}f'''(x_j)h^3 + \cdots .$$

Subtract to find the derivative $f'(x_j)$

$$f'(x_j) \approx \frac{f(x_{j+1}) - f(x_{j-1})}{2h}.$$

What is the order of accuracy?

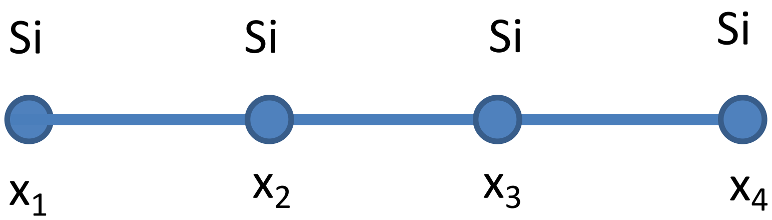
Summary: Finite Difference Method

- Meshing
- Defining input / output variables
- Defining operators
- Representing as a matrix equation
- Boundary conditions
- Sources of errors
- Testing for convergence

Finite Difference Method: Generalization (Two Different Media)

Homogneous Medium: Si

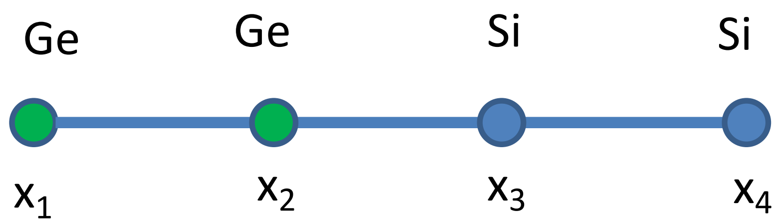
Dielectric constant: ϵ_{Si}



$$\nabla^2 V = -\frac{\rho}{\epsilon_{Si}}$$

Inhomogneous Medium: Ge, Si

Dielectric constant: $\epsilon_{Ge}, \epsilon_{Si}$



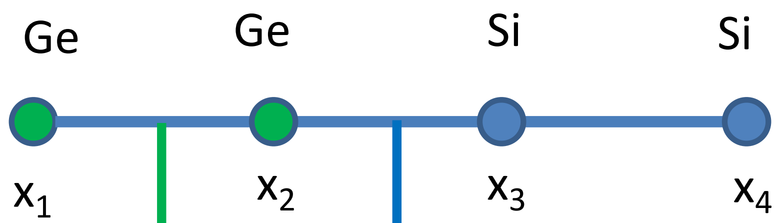
$$\nabla(\epsilon \nabla V) = -\rho$$

General form: $\epsilon(x)$

Finite Difference Method: Generalization (Two Different Media/Material)

Inhomogeneous Medium: Ge, Si

Dielectric constant: $\epsilon_{Ge}, \epsilon_{Si}$



$$\nabla(\epsilon \nabla V) = -\rho$$

General form: $\epsilon(x)$ $\quad (\nabla V)$

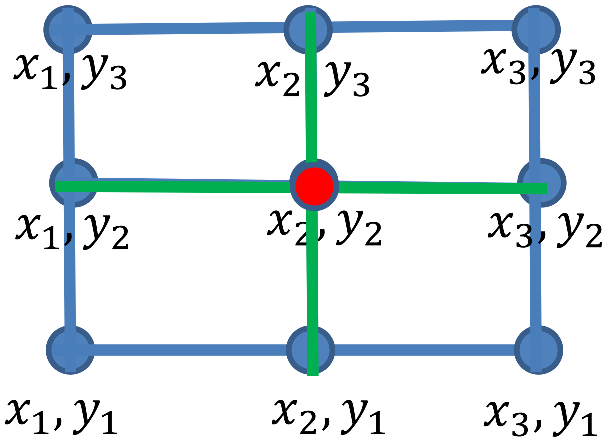
$$\frac{V_2 - V_1}{a} \qquad \frac{V_3 - V_2}{a}$$

Setting Dirichlet BC of
V=0 at the boundaries $\quad \nabla(\epsilon \nabla V)$

$$\frac{\frac{\epsilon_{Si}(V_3 - V_2)}{a} - \frac{\epsilon_{Ge}(V_2 - V_1)}{a}}{a}$$

$$\begin{bmatrix} -2\epsilon_{Ge} & \epsilon_{Ge} & 0 & 0 \\ \epsilon_{Ge} & -(\epsilon_{Ge} + \epsilon_{Si}) & \epsilon_{Si} & 0 \\ 0 & \epsilon_{Ge} & -(\epsilon_{Ge} + \epsilon_{Si}) & \epsilon_{Si} \\ 0 & 0 & \epsilon_{Si} & -2\epsilon_{Si} \end{bmatrix} \quad \frac{\epsilon_{Si} V_3 - (\epsilon_{Si} + \epsilon_{Ge}) V_2 + \epsilon_{Ge} V_1}{a^2}$$

Finite Difference Method: Generalization (2D Problems)



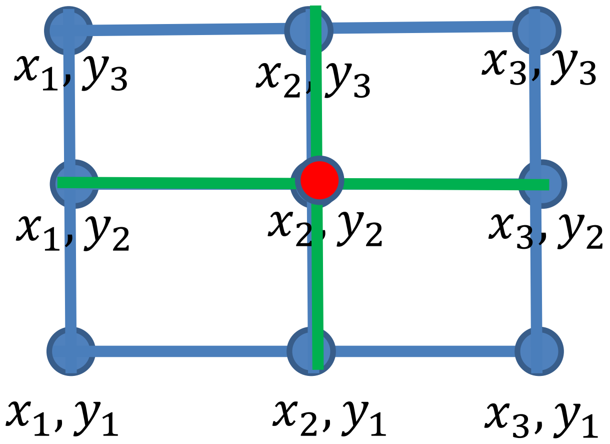
$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

$$\nabla^2 = \frac{d^2}{dx^2} + \frac{d^2}{dy^2}$$

$\frac{d^2}{dx^2}$	x_2, y_2	$V_{x_3,y_2} - 2V_{x_2,y_2} + V_{x_1,y_2}$	Horizontally
$\frac{d^2}{dy^2}$	x_2, y_2	$V_{x_2,y_3} - 2V_{x_2,y_2} + V_{x_2,y_1}$	Vertically
∇^2	x_2, y_2	$V_{x_3,y_2} + V_{x_2,y_3} - 4V_{x_2,y_2} + V_{x_1,y_2} + V_{x_2,y_1}$	

Diagonal elements (i,i) =-4, Off-diagonal elements 4 1's => 4 connections to nearest grid points

Finite Difference Method: Generalization (2D Problems)



$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

Assuming BC: V=0 at the edges

∇^2 x_2, y_2

$$V_{x_3,y_2} + V_{x_2,y_3} - 4V_{x_2,y_2} + V_{x_1,y_2} + V_{x_2,y_1}$$

$$
\begin{array}{c}
\begin{array}{ccc} \overbrace{\qquad\qquad\qquad}^{y_1} & \overbrace{\qquad\qquad\qquad}^{y_2} & \overbrace{\qquad\qquad\qquad}^{y_3} \end{array} \\
\begin{array}{c c}
\begin{array}{c} \\ y_1 \\ \\ \\ y_2 \\ \\ \\ y_3 \\ \\ \end{array} &
\begin{bmatrix}
-4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4
\end{bmatrix}
\end{array}
\end{array}
$$

Each 3x3 block is each horizontal row displaced in y.

Total Matrix: 3x3

(3 points in x & 3 points in y)

Generalization: Linear vs Non-linear Differential Equation

- In semiconductors, the left and right hand side of the Poisson equation are not independent.
- The charge density is a function of potential.
- Non-linear Poisson Equation

$$\nabla^2 V = -\frac{\rho(V)}{\epsilon}$$

Example:

$$\rho(V) \sim q N_C e^{(E_F - E_C + qV)/kT}$$

- Need to solve this iteratively with some initial guess for V.
- One method is Newton-Raphson.
- Define f(V) and find the root.

$$f(V) = \nabla^2 V + \frac{\rho(V)}{\epsilon}$$

Newton-Raphson technique of root finding

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

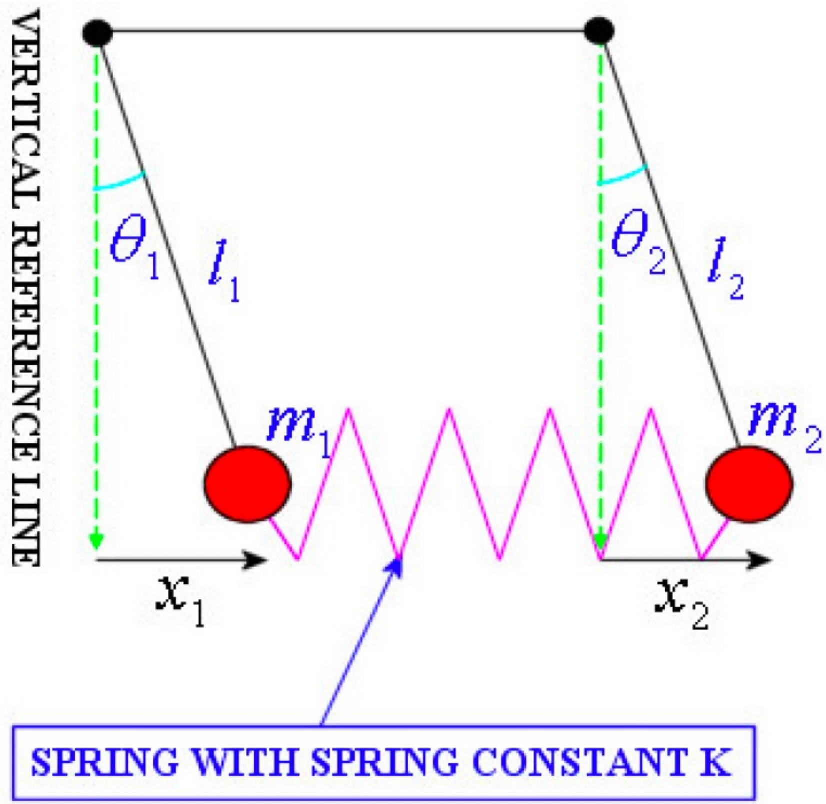
Generalization: Coupled Differential Equations

Example from your lab: Coupled Pendula

2 PDEs, solution of one depend
on the other and vice versa.

$$\ddot{\phi}_1(t) + A^2\phi_1\,(t) = -B^2[\phi_2(t) - \phi_1(t)],$$

$$\ddot{\phi}_2(t) + A^2\phi_2\,(t) = B^2[\phi_2(t) - \phi_1(t)].$$



Where A and B are constants; $\phi_1(t)$ and $\phi_2\,(t)$ are functions of time.

Generalization: Coupled Differential Equations

Example: Schrodinger-Poisson

Electrostatics

$$\nabla^2 V = -\frac{\rho}{\epsilon}$$

$$\Downarrow$$

$$V$$

ρ

V

Quantum Mechanics

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = E\psi$$

$$\Downarrow$$

$$\rho = q|\psi|^2$$

Self-consistent Solutions (Iterative)

Convergence: Both ρ and V are constant over iterations.

Summary: Generalizations

- Equations over heterogeneous domain
  (Poisson Eq. over two materials)

- 2 dimensions and more

- Non-linear differential equation (Non-linear Poisson)

- Coupled differential equations (Schrodinger-Poisson)