UNSW AUSTRALIA

Physics 3112: Experimental & Computational Physics

T1 2025

Never Stand Still | Science | School of Physics

Time Dependent PDEs

Differential Equations in Physics

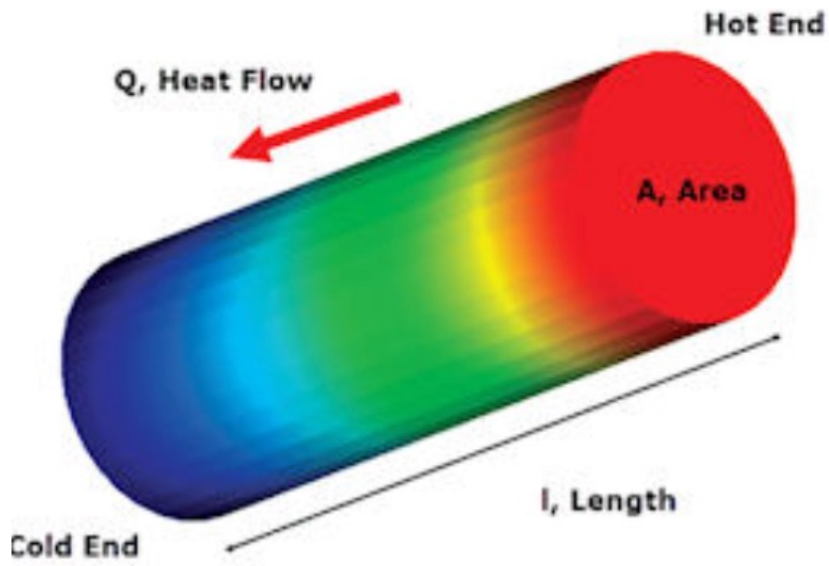
Thermal Physics: Heat Equation (2D)

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

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

Simplified Heat Equation

Assumptions:

- 1D
- q=0

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

Solution: $T(t,x) \rightarrow T_{t_i,x_j}$

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

$$\frac{T_{t_{i+1},x_j} - T_{t_i,x_j}}{\Delta t}$$

At each x_j

$$\alpha \frac{T_{t_i,x_{j+1}} - 2T_{t_i,x_j} + T_{t_i,x_{j-1}}}{(\Delta x)^2}$$

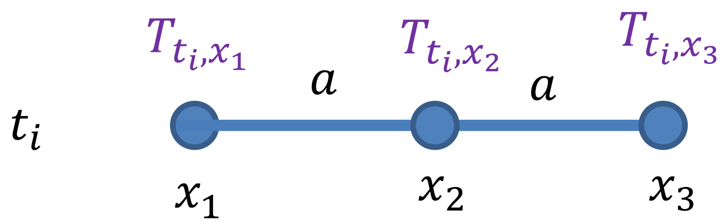
At each t_i

Space

- Mesh/Discretization
- Finite Difference
- Boundary value problem (Boundary conditions)

Time

- Time stepping Δt
- Initial condition ($t = 0$)



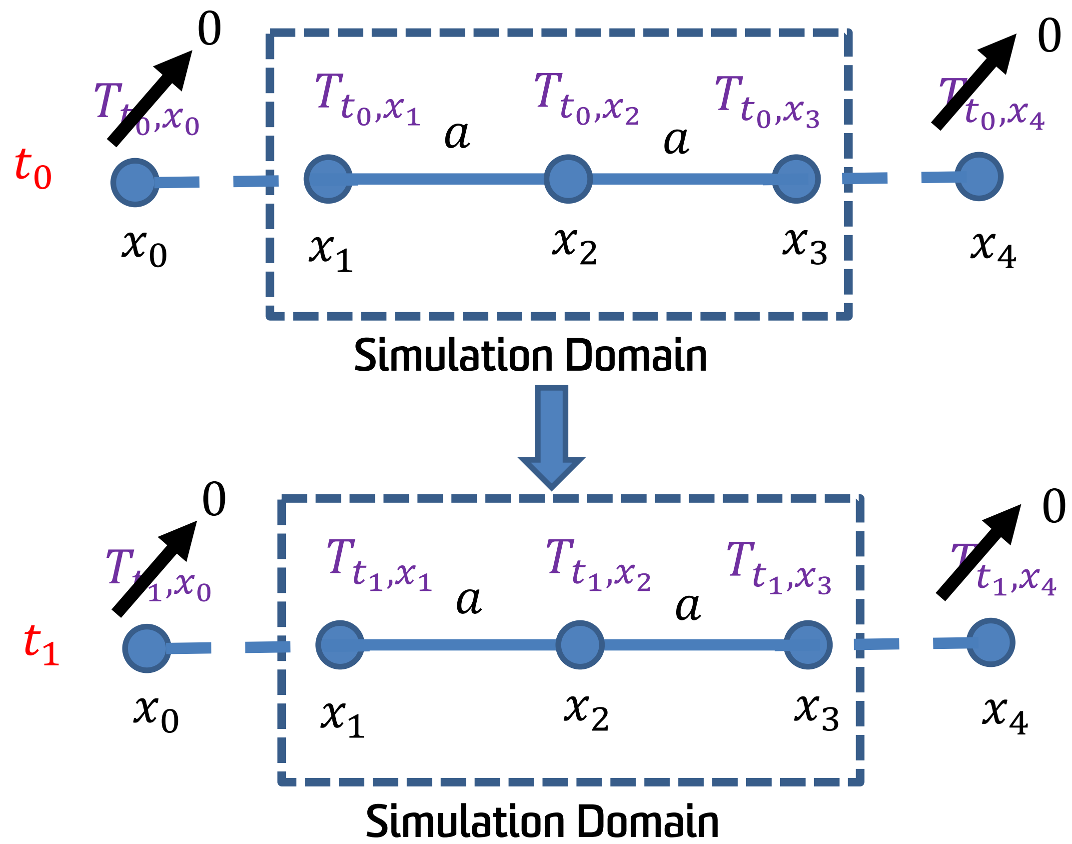
Demonstration:

1. Solve over 3 spatial points (x_1, x_2, x_3)
2. Solve over 2 temporal points (t_1, t_2)
3. Initial condition: $T(t_0, x) \rightarrow T_{t_0,x_1}, T_{t_0,x_2}, T_{t_0,x_3}$
4. Boundary condition: $T(t, x_{BC}) \rightarrow T_{t,x_0} = T_{t_0,x_4} = 0$

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

$$\frac{T_{t_{i+1},x_j} - T_{t_i,x_j}}{\Delta t} = \alpha \frac{T_{t_i,x_{j+1}} - 2T_{t_i,x_j} + T_{t_i,x_{j-1}}}{(\Delta x)^2}$$

$$T_{t_{i+1},x_j} = T_{t_i,x_j} + \Delta t \alpha \frac{T_{t_i,x_{j+1}} - 2T_{t_i,x_j} + T_{t_i,x_{j-1}}}{(\Delta x)^2}$$



$$\begin{bmatrix} T_{t_1,x_1} \\ T_{t_1,x_2} \\ T_{t_1,x_3} \end{bmatrix} = \begin{bmatrix} T_{t_0,x_1} \\ T_{t_0,x_2} \\ T_{t_0,x_3} \end{bmatrix} + \frac{\alpha \Delta t}{a^2} \begin{bmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} T_{t_0,x_1} \\ T_{t_0,x_2} \\ T_{t_0,x_3} \end{bmatrix}$$

Next t_2

Forward time stepping

- Unstable
- Works better if $\frac{\alpha \Delta t}{a^2} \ll 1$

Crank-Nicolson Method

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

1st order in time

$$\frac{T_{t_{i+1},x_j} - T_{t_i,x_j}}{\Delta t} = \alpha \frac{T_{t_i,x_{j+1}} - 2T_{t_i,x_j} + T_{t_i,x_{j-1}}}{(\Delta x)^2}$$

$$\frac{T_{t_{i+1},x_j} - T_{t_i,x_j}}{\Delta t} = \alpha \frac{1}{2}\left[\frac{T_{t_i,x_{j+1}} - 2T_{t_i,x_j} + T_{t_i,x_{j-1}}}{(\Delta x)^2} + \frac{T_{t_{i+1},x_{j+1}} - 2T_{t_{i+1},x_j} + T_{t_{i+1},x_{j-1}}}{(\Delta x)^2}\right]$$

$$r = \frac{\alpha \Delta t}{2(\Delta x)^2}$$

$$-rT_{t_{i+1},x_{j+1}} + (1+2r)T_{t_{i+1},x_j} - rT_{t_{i+1},x_{j-1}} = rT_{t_i,x_{j+1}} + (1-2r)T_{t_i,x_j} + rT_{t_i,x_{j-1}}$$

$$\begin{bmatrix} 1+2r & -r & 0 \\ -r & 1+2r & -r \\ 0 & -r & 1+2r \end{bmatrix} \begin{bmatrix} T_{t_{i+1},x_1} \\ T_{t_{i+1},x_2} \\ T_{t_{i+1},x_3} \end{bmatrix} = \begin{bmatrix} 1-2r & r & 0 \\ r & 1-2r & r \\ 0 & r & 1-2r \end{bmatrix} \begin{bmatrix} T_{t_i,x_1} \\ T_{t_i,x_2} \\ T_{t_i,x_3} \end{bmatrix}$$

Caution: Always avoid matrix inversion!!

Here, use tridiagonal algorithm: https://en.wikipedia.org/wiki/Tridiagonal_matrix_algorithm

Why Crank-Nicolson? 2nd order in time, Usually more stable! Here, use:

numpy.linalg.solve

```
linalg.solve(a, b)
```

numpy.linalg.solve

`linalg.solve(a, b)` [source]

Solve a linear matrix equation, or system of linear scalar equations.

Computes the “exact” solution, *x*, of the well-determined, i.e., full rank, linear matrix equation *ax* = *b*.

Parameters: **a : *(..., M, M) array_like***

Coefficient matrix.

b : *{(..., M,), (..., M, K)}, array_like*

Ordinate or “dependent variable” values.

Returns: **x : *{(..., M,), (..., M, K)} ndarray***

Solution to the system a x = b. Returned shape is identical to *b*.

Raises: **LinAlgError**

If *a* is singular or not square.

https://numpy.org/doc/stable/reference/generated/numpy.linalg.solve.html

Examples

Solve the system of equations `x0 + 2 * x1 = 1` and `3 * x0 + 5 * x1 = 2`:

```
>>> a = np.array([[1, 2], [3, 5]])
>>> b = np.array([1, 2])
>>> x = np.linalg.solve(a, b)
>>> x
array([-1.,  1.])
```

Convection-Diffusion equation (Stat. Mech., solid-state devices, biophysics)

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \nabla c - \mathbf{v} c) + R$$

c is some quantity (Temperature in heat equation, mass or charge concentration, etc)

D is the diffusion coefficient

v is the velocity of flow

R is a source or sink term

Continuity equation

$$\frac{\partial c}{\partial t} + \nabla \cdot \mathbf{j} = R,$$

$$\mathbf{j}_{\mathrm{diff}} = -D \nabla c$$

(Fick's Law)

$$\mathbf{j}_{\mathrm{adv}} = \mathbf{v} c$$

$$\mathbf{j} = \mathbf{j}_{\mathrm{diff}} + \mathbf{j}_{\mathrm{adv}} = -D \nabla c + \mathbf{v} c.$$

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

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

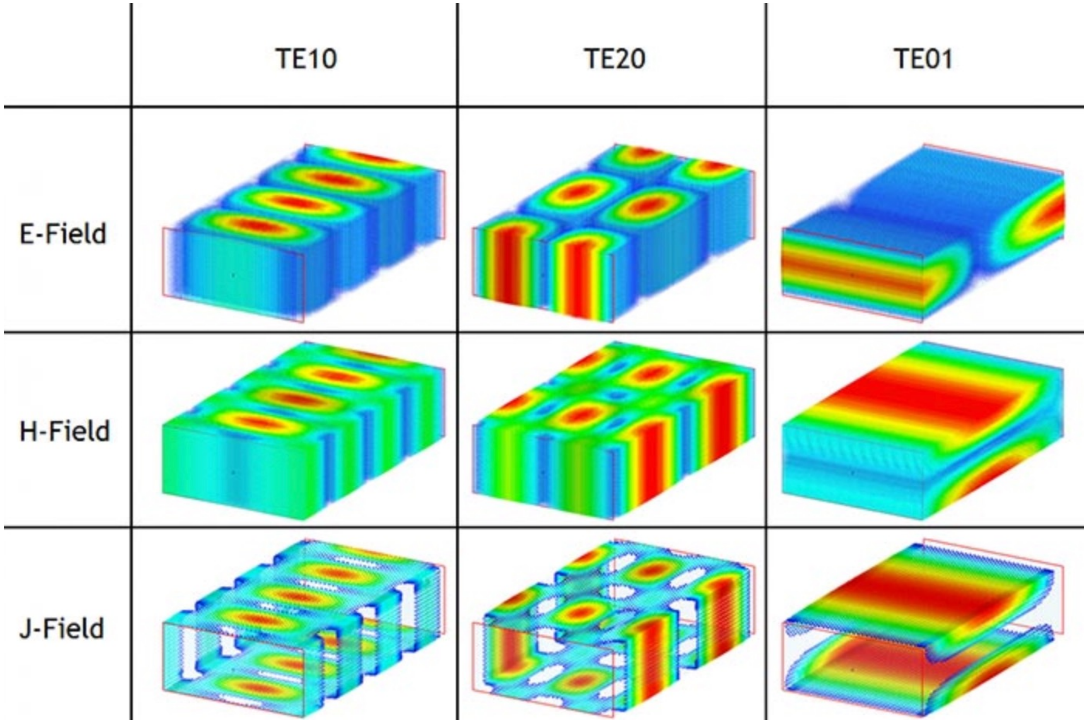
$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\boldsymbol{B} = \mu \boldsymbol{H}$$

$$\boldsymbol{D} = \epsilon \boldsymbol{E}$$

$$\nabla \times \boldsymbol{E} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ E_x & E_y & E_z \end{vmatrix}$$

Wave Guides



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

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

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

Finite Difference Time Domain (FDTD)

Example $\boldsymbol{E} = (E_x, 0,0)$ $\boldsymbol{B} = (0, B_y, 0)$ $\boldsymbol{J} = (0,0,0)$

E-field

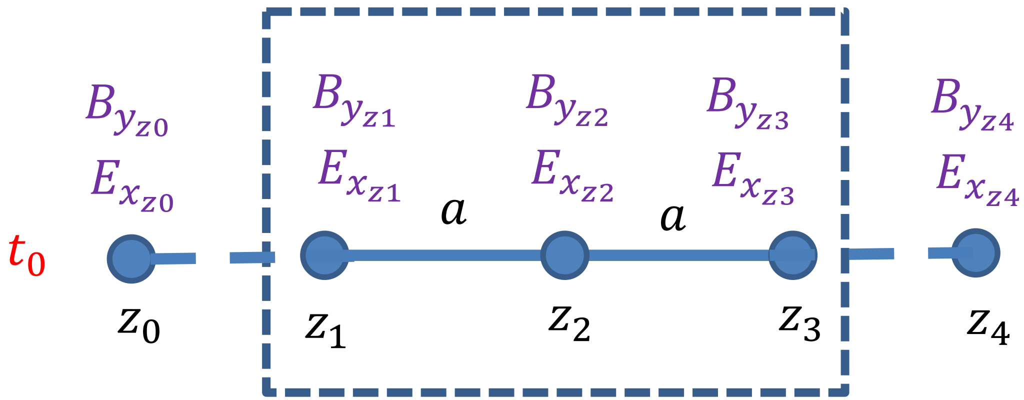
$$\nabla\times\boldsymbol{E} = \frac{\partial E_x}{\partial z}\mathbf{j} - \frac{\partial E_x}{\partial y}\boldsymbol{k} = \frac{\partial B_y}{\partial t}\boldsymbol{j} + \cancelto{0}{\frac{\partial B_z}{\partial t}}\boldsymbol{k}$$

B-field

$$\nabla\times\boldsymbol{B} = -\frac{\partial B_y}{\partial z}i + \frac{\partial B_y}{\partial x}\boldsymbol{k} = \frac{\mu}{\epsilon}\left(\frac{\partial E_x}{\partial t}\boldsymbol{i} + \cancelto{0}{\frac{\partial E_z}{\partial t}}\boldsymbol{k}\right)$$

$$\frac{\partial E_x}{\partial z} = \frac{\partial B_y}{\partial t} \qquad -\frac{\partial E_x}{\partial y} = 0$$

$$-\frac{\partial B_y}{\partial z} = \frac{\mu}{\epsilon}\frac{\partial E_x}{\partial t} \qquad \frac{\partial B_y}{\partial x} = 0$$



Simulation Domain

- Coupled PDEs
- Boundary conditions on E_x and B_y
- Initial conditions at t_0 on E_x and B_y

Maxwell's Equations by FDTD

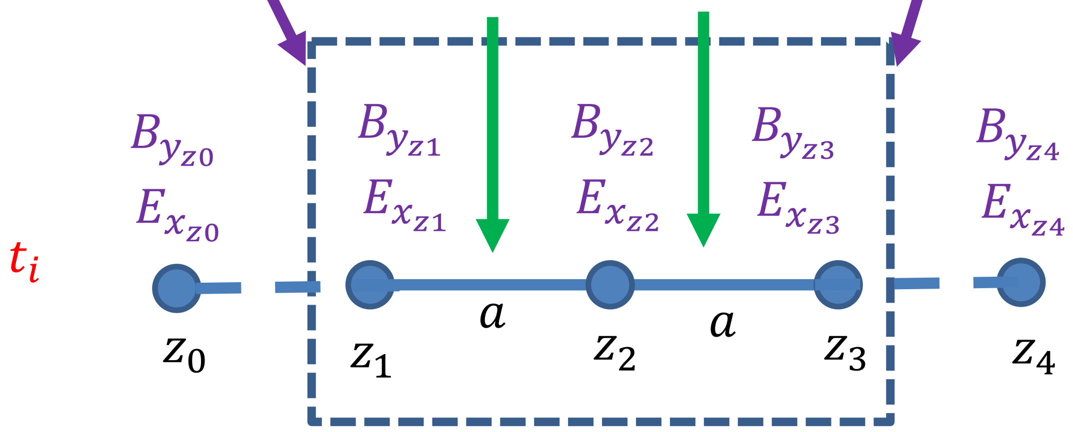
Iteration

$$\frac{\partial E_x}{\partial z} = \frac{\partial B_y}{\partial t} \rightarrow \frac{B_{y\,t_{i+1}} - B_{y\,t_i}}{\Delta t}$$

$$-\frac{\partial B_y}{\partial z} = \frac{\mu}{\epsilon}\frac{\partial E_x}{\partial t} \rightarrow \frac{E_{x\,t_{i+1}} - E_{x\,t_i}}{\Delta t}$$

$$\frac{B_{y\,z_2} - B_{y\,z_1}}{a} \qquad \frac{B_{y\,z_3} - B_{y\,z_2}}{a}$$

$$\frac{E_{x\,z_2} - E_{x\,z_1}}{a} \qquad \frac{E_{x\,z_3} - E_{x\,z_2}}{a}$$



Simulation Domain

Finite Difference:
Forward Difference

- Stability
- Error

Open Boundary Condition

- Also known as absorbing boundary condition or reflecting boundary condition
- Prevent infinite reflections from simulation domain boundaries

Time dependent Schrodinger Equation

Using TDSE we will calculate the wavefunction in the next timestep $\psi(t + \Delta t)$ based on the value in the current/previous timestep $\psi(t)$.

To discretize the TDSE we will use Crank-Nicolson scheme (https://en.wikipedia.org/wiki/Crank%E2%80%93Nicolson_method):

$$i\hbar \frac{\psi(t+\Delta t) - \psi(t)}{\Delta t} = \frac{1}{2}[H(t+\Delta t)\psi(t+\Delta t) + H(t)\psi(t)]$$

When we move all the $(t + \Delta t)$ terms to the left and t terms to the right we get:

$$\left[1 + \frac{i\Delta t}{2\hbar} H(t+\Delta t)\right]\psi(t+\Delta t) = \left[1 - \frac{i\Delta t}{2\hbar\Delta t} H(t)\right]\psi(t)$$

We will start from some initial value $\psi(t = 0)$ and calculate each next timestep with this equation. Note that the only thing unknow in this equation is vector $\psi(t + \Delta t)$. The terms in paratheses are matrices. 1 stands for identity matrix (of the same size as our problem,) and you can calculate Hamiltonian matrix for any moment in time, as the only time-dependent part is the electric field and you have exact formula for that.

So if you name the matrix $A = \left[1 + \frac{i\Delta t}{2\hbar} H(t+\Delta t)\right]$, and the vector $B = \left[1 - \frac{i\Delta t}{2\hbar\Delta t} H(t)\right]\psi(t)$ (you know $\psi(t)$ so can multiply the matrix in the parenthesis with $\psi(t)$ obtaining a vector) you will be solving $A\psi(t + \Delta t) = B$ matrix equation. This can be done with Python function: **numpy.linalg.solve(A,B).** As a result you will get vector $\psi(t + \Delta t)$.

TDSE Crank Nicholson Algorithm

- Initialize the system: calculate $H(t=0)$ and set initial state $\psi(t=0)$ as the ground state of this Hamiltonian
- Loop over time with timestep Δt, and in each iteration:
  - update V$(t+\Delta t)$
  - calculate $H(t+\Delta t)$ with updated V
  - solve the $A\psi(t+\Delta t)=B$ equation
  - update $\psi(t) \coloneqq \psi(t+\Delta t)$ and $H(t) \coloneqq H(t+\Delta t)$ for the new iteration

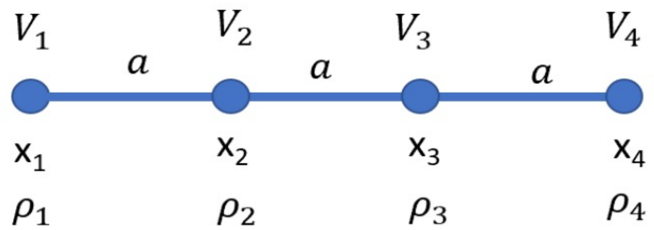
Note: as you might notice, you will need to keep 2 matrices for Hamiltonian (e.g. H and H_new) and two vectors for the wavefunction (e.g. psi and psi_new) and update them in every iteration to be able to solve the discretized equation.

Summary: Time Dependence

- Time Dependent Problems through Time Stepping
- Initial Conditions, Forward Time Derivatives
- Example: 1D Heat Equation
- Stability and Error
- Crank Nicolson Method
- Maxwell's Equation: Finite Difference Time Domain

Quiz 5 Discussion

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



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

A 1D Poisson equation is to be solved over the 4 points in a grid using the finite difference technique. V_i and ρ_i are the voltages and charge densities on grid point i, and ε is the dielectric constant of the medium. The matrix representation of this equation is shown on the right. Next 5 questions are based on this system.

What are the values of the constants (A, B, C, D, E) for each of the following cases?

Q1

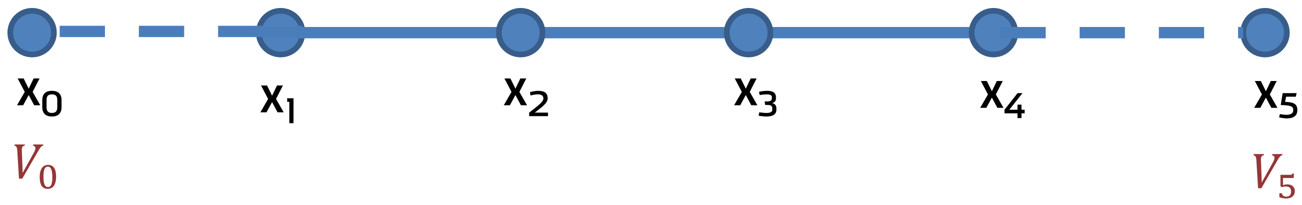
The left and right boundary voltages outside the grid are set to V_0 and 0 respectively.

- a. $(-2, 0, -2, 0, V_0)$
- b. $(-2, -2, 0, V_0, 0)$
- c. $(-1, -1, 0, V_0, 0)$
- d. I don't know
- e. $(-2, -2, 0, 0, V_0)$

Recap here: Numerical Solution of Differential Equations: The Finite Difference Method

Step 5: Boundary conditions (2 common types)

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



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

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

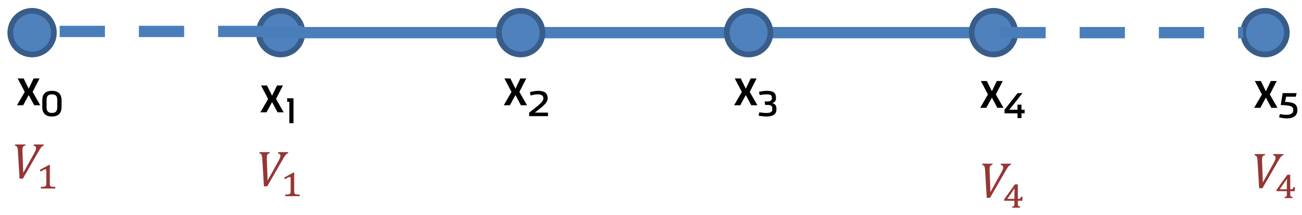
x_4 $\quad V_5 - 2V_4 + V_3 = -\rho_4 a^2/\epsilon \qquad -2V_4 + V_3 = -\rho_4 a^2/\epsilon - V_5$

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

Numerical Solution of Differential Equations: The Finite Difference Method

Step 5: Boundary conditions (2 common types)

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



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

$E = -\nabla V$ Constant

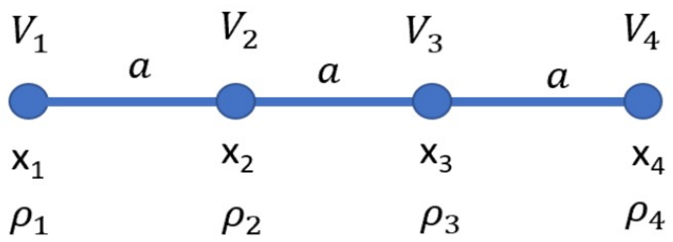
Example: Set E=0 at the edges

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

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

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

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



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

A 1D Poisson equation is to be solved over the 4 points in a grid using the finite difference technique. V_i and ρ_i are the voltages and charge densities on grid point i, and ε is the dielectric constant of the medium. The matrix representation of this equation is shown on the right. Next 5 questions are based on this system.

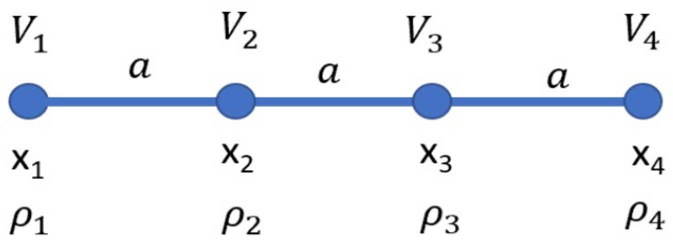
What are the values of the constants (A, B, C, D, E) for each of the following cases?

Q2

The left and right boundary electric fields are set to zero.

- a. $(-2, -2, 0, 0, 0)$
- b. $(-2, 0, -2, 1, 1)$
- c. $(-1, -1, 0, 1, 1)$
- d. I don't know
- e. $(-1, -1, 0, 0, 0)$

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



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

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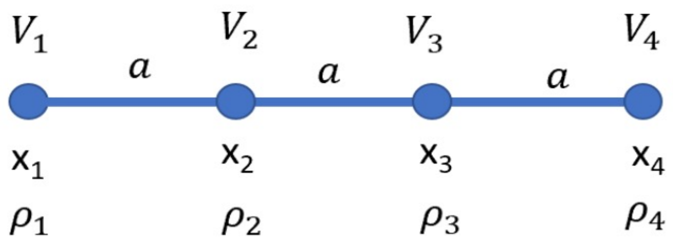
What are the values of the constants (A, B, C, D, E) for each of the following cases?

Q3

The left boundary electric field is set to zero and the right boundary voltage is set to V_0.

- a. $(-2, -2, 0, 0, V_0)$
- b. $(-1, -2, 0, 0, V_0)$
- c. I don't know
- d. $(-1, -1, 0, 0, V_0)$
- e. $(-2, -2, 0, V_0, 0)$

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



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

A 1D Poisson equation is to be solved over the 4 points in a grid using the finite difference technique. V_i and ρ_i are the voltages and charge densities on grid point i, and ε is the dielectric constant of the medium. The matrix representation of this equation is shown on the right. Next 5 questions are based on this system.

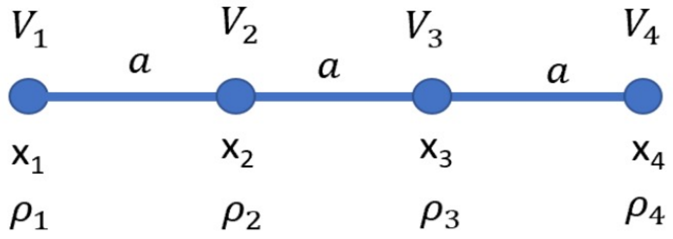
What are the values of the constants (A, B, C, D, E) for each of the following cases?

Q4

Periodic boundary conditions are used (the leftmost value of the potential is the same as the rightmost value over the domain of grid points).

- a. I don't know
- b. $(-1, -1, 2, 0, 0)$
- c. $(-2, -2, 1, 0, 0)$
- d. $(-2, -2, 0, V_0, V_0)$
- e. $(-2, -2, 0, 1, 1)$

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



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

A 1D Poisson equation is to be solved over the 4 points in a grid using the finite difference technique. V_i and ρ_i are the voltages and charge densities on grid point i, and ε is the dielectric constant of the medium. The matrix representation of this equation is shown on the right. Next 5 questions are based on this system.

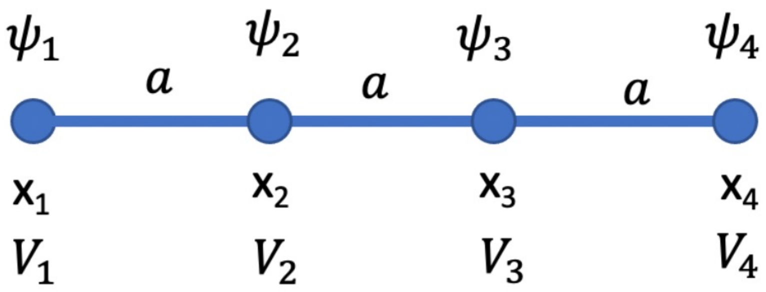
What are the values of the constants (A, B, C, D, E) for each of the following cases?

Q5

What is the 1^{st} order central difference at node 2?

- a. $\frac{V_3 - V_2}{a}$
- b. $\frac{V_3 - V_1}{2a}$
- c. I don't know
- d. $\frac{V_2 - V_1}{a}$
- e. $\frac{V_3 - 2V_2 + V_1}{a^2}$

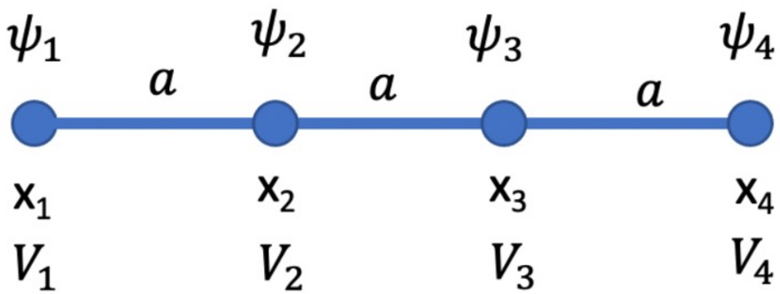
$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \mathrm{E}\begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

A one-dimensional Schrodinger equation in a solid material is to be solved over the 4 points (nodes) in a uniformly spaced grid of spacing a shown above using the finite difference technique. ψ_i and V_i are the wavefunction and potential energy on grid point i respectively. m^* is the electron effective mass in the material. The matrix representation of this equation is shown on the right in the figure above, where a_{ij} is the matrix element corresponding to i-th row and j-th column. The matrix is Hermitian ($a_{ij} = a_{ji}^*$). Unless otherwise stated, assume closed boundary conditions at the ends of this grid (i.e. wavefunction assuming zero value). The next 5 questions are based on the above setup.

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \mathrm{E} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

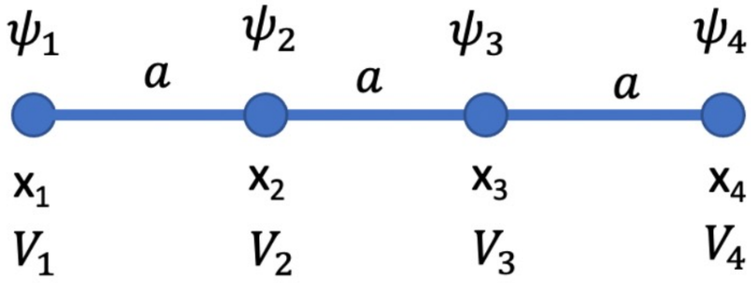
Q6

What is the value of the matrix element a_{12}?

Select one:

- a. $\frac{\hbar^2}{m^* a^2} + V_1$
- b. $\frac{\hbar^2}{2m^* a^2}$
- c. $\frac{\hbar^2}{2m^*}$
- d. $-\frac{\hbar^2}{2m^* a^2}$
- e. $\frac{\hbar^2}{2m^* a^2} + V_1$

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x)$$



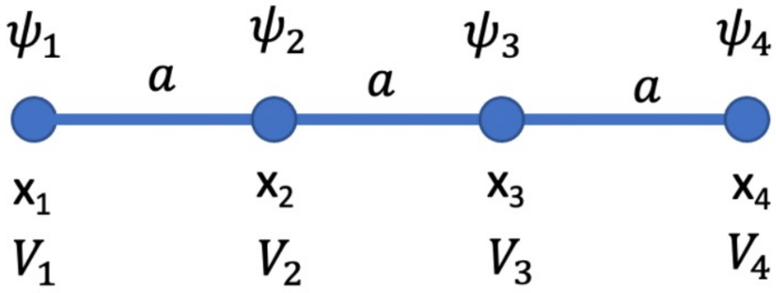
$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{bmatrix} = \mathrm{E}\begin{bmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{bmatrix}$$

Q7

What is the value of the matrix element a_{11}?

- a. $\frac{\hbar^2}{m^* a^2} + V_1$
- b. $-\frac{\hbar^2}{2m^* a^2} + V_1$
- c. $\frac{\hbar^2}{2m^* a^2}$
- d. $\frac{\hbar^2}{2m^* a^2} + V_1$
- e. $\frac{\hbar^2}{2m^*} + V_1$

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$



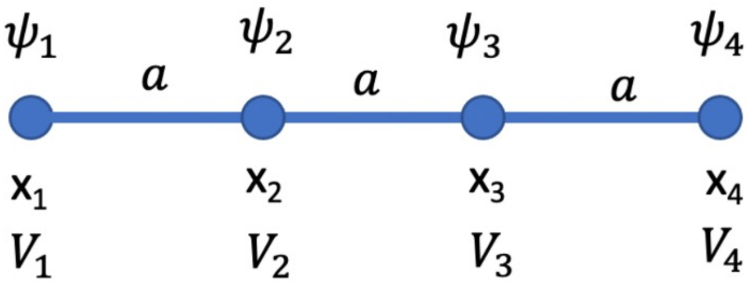
$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \mathrm{E} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

Q8

What is the value of the matrix element a_{14}?

- a. 0
- b. 1
- c. $-\frac{\hbar^2}{2m^* a^2}$
- d. $\frac{\hbar^2}{m^* a^2}$
- e. $\frac{\hbar^2}{2m^* a^2}$

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$



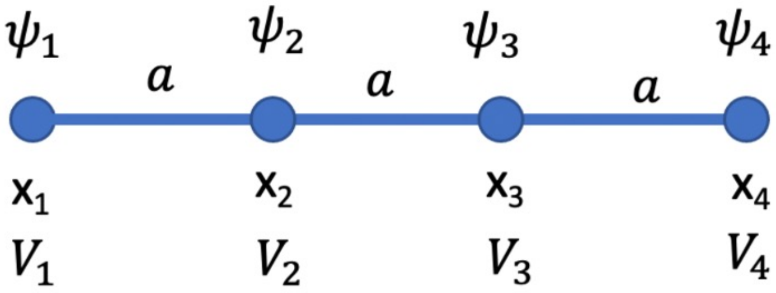
$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \mathrm{E} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

Q9

If periodic boundary conditions are used at the ends of the grid, what is the value of the modified matrix element from the previous question?

- a. $\frac{\hbar^2}{2m^* a^2}$
- b. $-\frac{\hbar^2}{2m^* a^2}$
- c. $\frac{\hbar^2}{m^* a^2} + V_1$
- d. $-\frac{\hbar^2}{m^* a^2}$
- e. $\frac{\hbar^2}{m^* a^2} + V_1 + V_4$

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$$



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix} = \mathrm{E} \begin{bmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{bmatrix}$$

Q10

If Neumann boundary condition is used at the left boundary with the condition that $\frac{d\psi}{dx} = 0$ to the left of node 1, what is the new value of a_{11}?

- a. $\frac{\hbar^2}{2m^* a^2} - V_1$
- b. $-\frac{\hbar^2}{2m^* a^2}$
- c. $\frac{\hbar^2}{2m^* a^2} + V_1$
- d. $\frac{\hbar^2}{m^* a^2} + V_1$
- e. $\frac{\hbar^2}{2m^* a^2}$