

## Section 18 Semiconductor Equations

Gerhard Klimeck

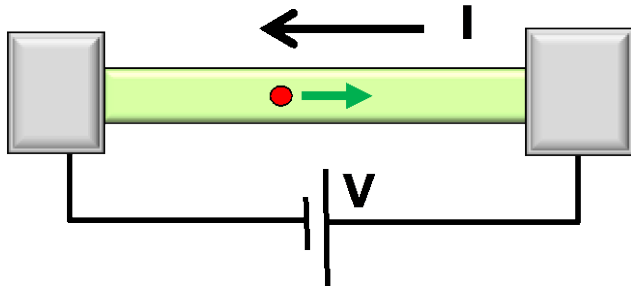
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School of Electrical and  
Computer Engineering

# Section 18

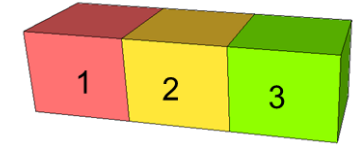
## Continuity Equations



$$I = G \times V$$

$$= q \times n \times v \times A$$

↑ charge density    ↑ velocity    area



- 18.1 Continuity Equations
- 18.2 Analytical Solutions (Strategy & Examples)
- 18.3 Numerical Solutions
  - » Basic Transport Equations
  - » Gridding and finite differences
  - » Discretizing equations and boundary conditions
  - » Iterative Solution Approach

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N$$

$$\mathbf{J}_N = qn\mu_N E + qD_N \nabla n$$

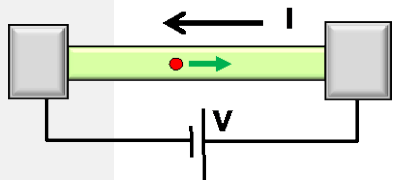
$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_P - r_P + g_P$$

$$\mathbf{J}_P = qp\mu_P E - qD_P \nabla p$$

$$\nabla \cdot D = q(p - n + N_D^+ - N_A^-)$$

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# Now the Continuity Equations ...



$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N$$

Continuity eqn. for electrons

$$\mathbf{J}_N = qn\mu_N \mathbf{E} + qD_N \nabla n$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_P - r_P + g_P$$

Continuity eqn. for holes

$$\mathbf{J}_P = qp\mu_P \mathbf{E} - qD_P \nabla p$$

$$\nabla \cdot \mathbf{D} = q(p - n + N_D^+ - N_A^-)$$

Poisson equation

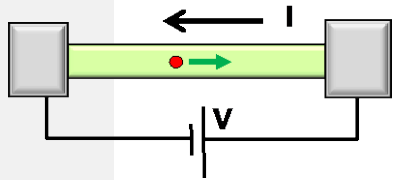
These equations have been state of the art in device modeling until 'recently' (20 years ago...)

Nano-scaled Devices – Non-Equilibrium Green Functions (NEGF)

Theory for Electrical Engineers: Supriyo Datta (Purdue)

NEGF Simulation Tools for atomistic devices: NEMO - Klimeck

# Some critical remarks about these equations



- Continuity equations are *always* valid (regardless of the detailed physical model describing the device) because they describe a conservation law.

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N \quad \frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_P - r_P + g_P$$

- **Poisson equation** as given does not account for explicit electron-electron repulsion. Might need to be modified for strongly correlated systems.

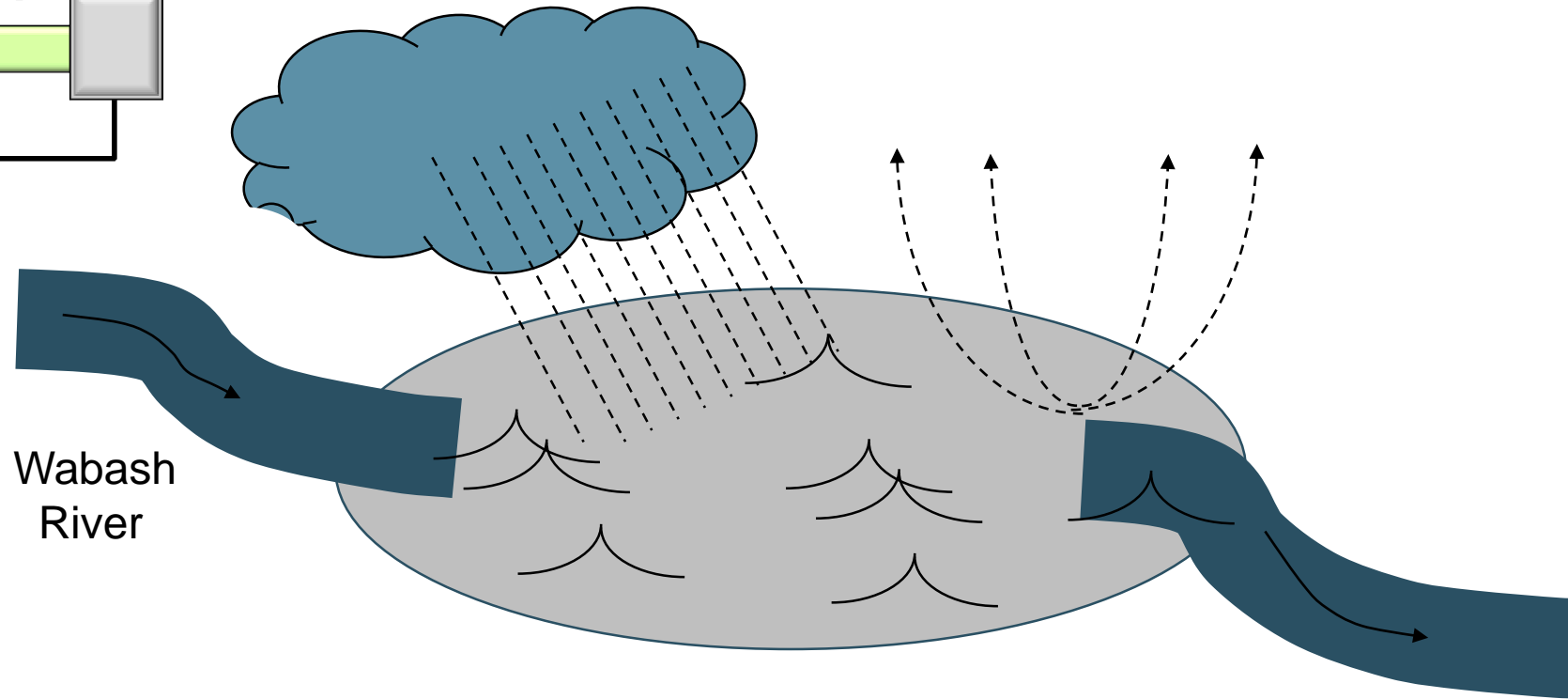
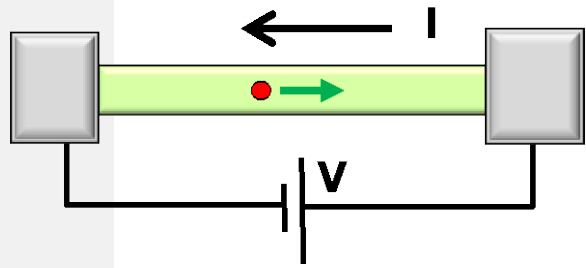
$$\nabla \cdot \mathbf{D} = q(p - n + N_D^+ - N_A^-)$$

- **Drift and Diffusion equations** get modified when devices are so small that essentially no scattering takes place within the device.

$$\mathbf{J}_N = qn\mu_N E + qD_N \nabla n$$

$$\mathbf{J}_P = qp\mu_P E - qD_P \nabla p$$

# Continuity Equation prequel: A Good Analogy



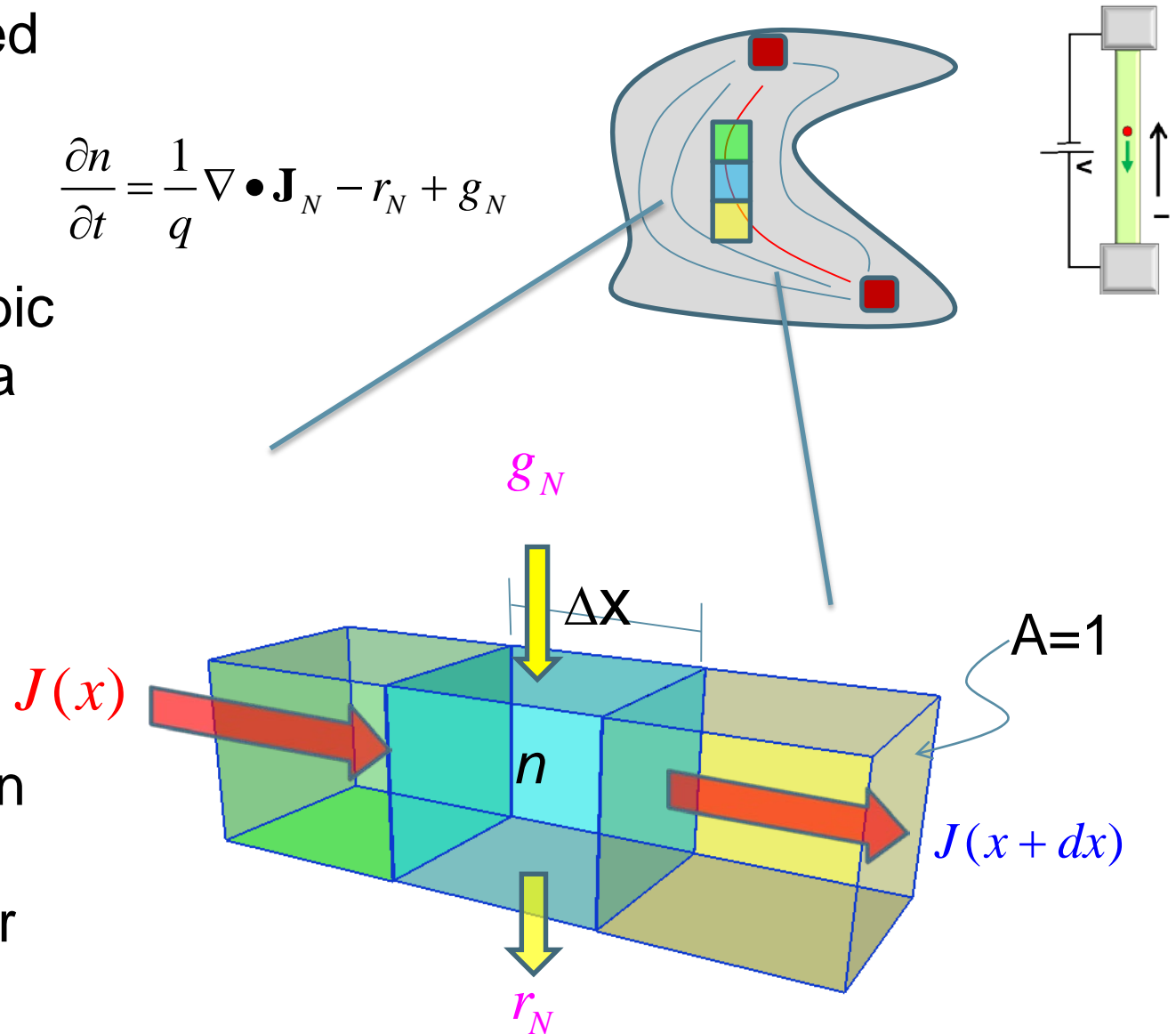
Rate of increase of  
water level in lake = (in flow - outflow) + rain - evaporation

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N$$

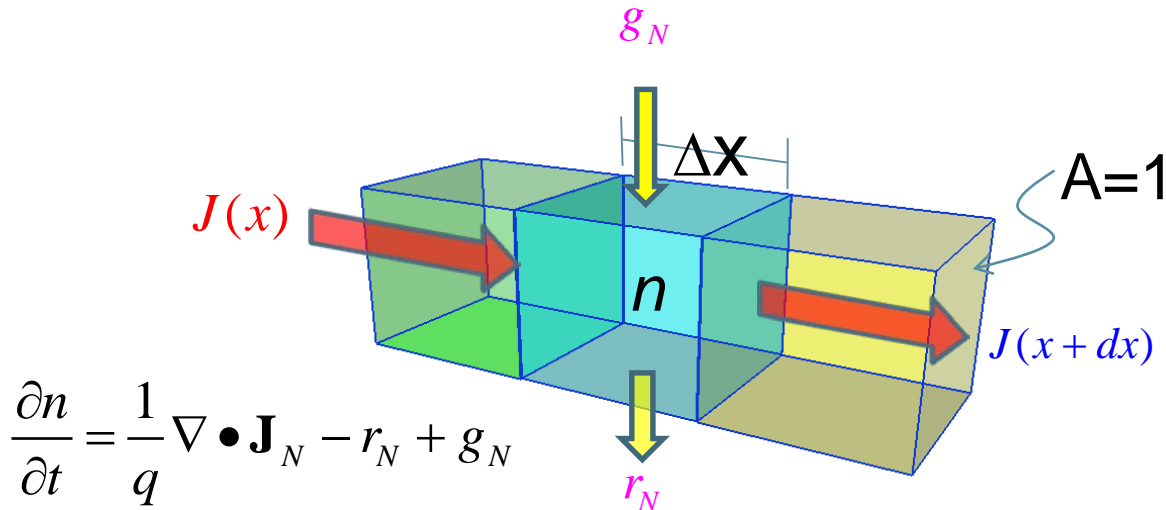
# Now the Continuity Equations for electrons...

- Consider an arbitrarily shaped semiconductor with contacts that pump in current.
- Divide this arbitrary semiconductor into small cubic boxes of cross sectional area 'A' and length  $\Delta x$ .
- Boxes are large enough that concepts like effective mass, mobility etc. are valid inside these boxes.
- Electrons coming in are given by  $J(x)$ , going out  $\rightarrow J(x+\Delta x)$
- Total number of electrons per  $\text{cm}^3 \rightarrow n$

$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N$$



# Now the Continuity Equations ...

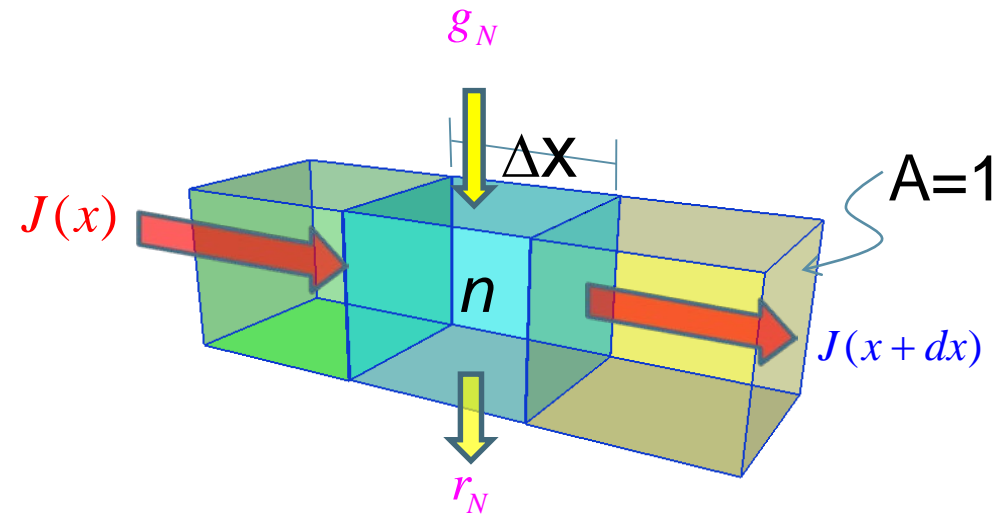


$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N$$

- $g_N$  → generation rate in (per  $\text{cm}^3$  per sec) from external processes such as light.
- $r_N$  → recombination rate in (per  $\text{cm}^3$  per sec) in the central box.

- We wish to relate all of these factors that affect the concentration of carriers in the central box.
- Our strategy (remember the analogy)– The *rate* of change of number of electrons INSIDE the central box should be equal to
  - No. of electrons coming in MINUS No. of electrons going out per sec (governed by current density  $J(x)$  and  $J(x+\Delta x)$ ) PLUS
  - No. of electrons getting generated from external processes per sec (governed by generation rate  $g_N$ ) MINUS
  - No. of electrons lost by recombination per sec (governed by recombination rate  $r_N$ )

Let's just write the equations down...



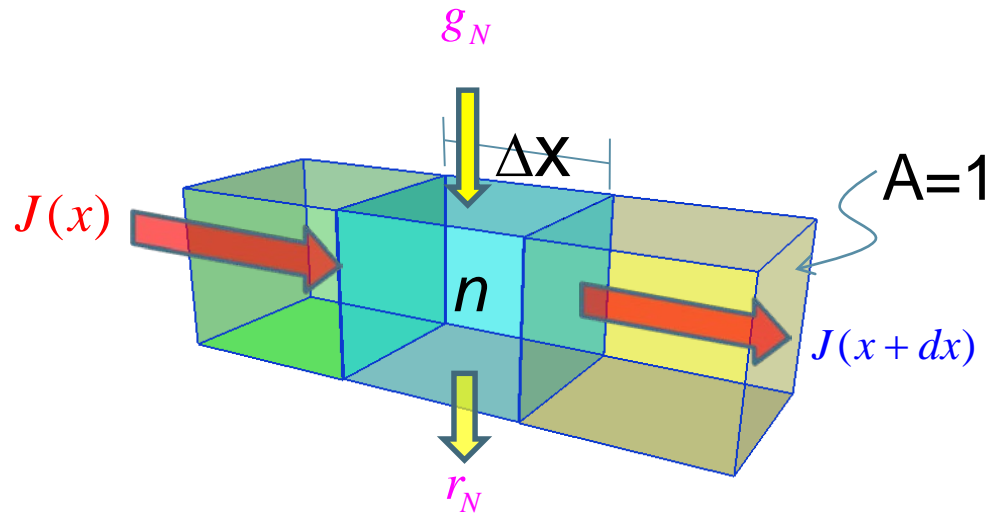
$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N$$

$$\frac{\partial (A \times \Delta x \times n)}{\partial t} = \frac{A \times J_n(x) - A \times J_n(x+dx)}{-q} + A \times g_N \Delta x - A \times r_N \Delta x$$

$$\frac{\partial n}{\partial t} = \frac{J_n(x) - J_n(x+dx)}{-q \Delta x} + g_N - r_N = \frac{1}{q} \nabla \cdot \mathbf{J}_n + g_N - r_N$$

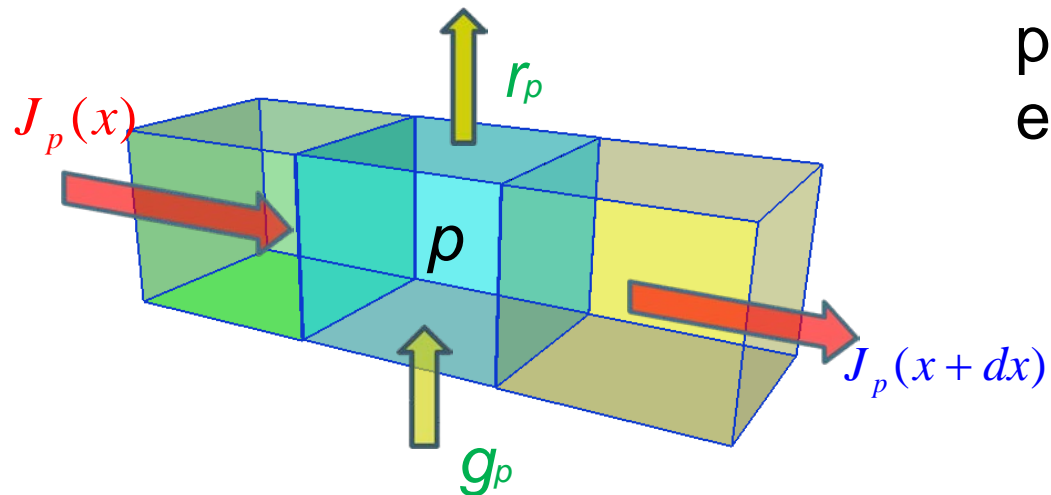


# Continuity Equations for Electron/Holes



$$\frac{\partial n}{\partial t} = \frac{1}{q} \nabla \cdot \mathbf{J}_N - r_N + g_N$$

Usually generation and recombination rates for electrons and holes are the same since the same processes create/destroy an electron/hole



$$\frac{\partial p}{\partial t} = -\frac{1}{q} \nabla \cdot \mathbf{J}_P + g_P - r_P$$

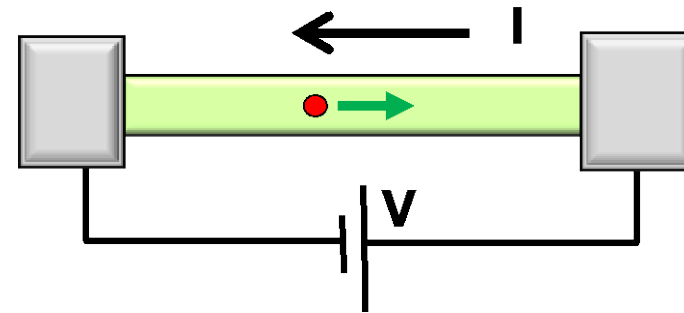
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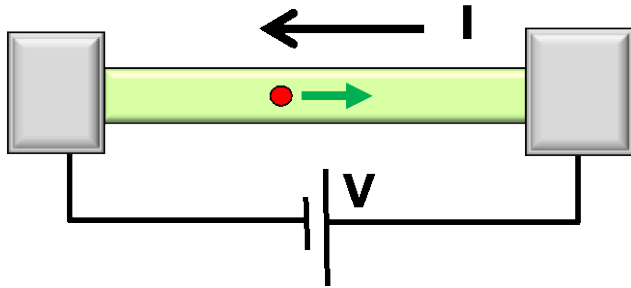
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Two methods of solution:

Numerical and Analytical

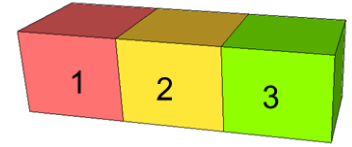
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charge density velocity area



## • 18.1 Continuity Equations

## • 18.2

## • 18.3

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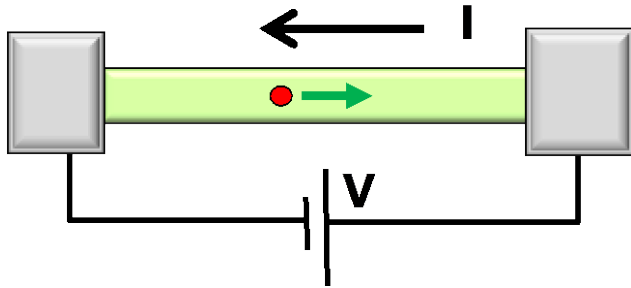
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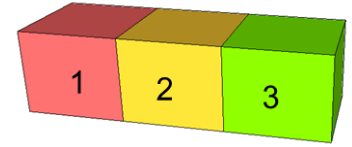
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