Chapter 5

Potentials and Fields

5.1 Laplace's equation for electric potential

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = 0$$

Eq. (5.1)

Partial differential equation (PDE)

- $V = V(x,y,z)$ electric potential in a region of space that do not contain any electric charges
- Different from previous cases: here boundary conditions are needed in place of initial conditions.

no comparable "general purpose" algorithms for PDEs.

elliptic equations → **relaxation method**

Note: this is a 2-D motion

Discretisation

$x = i\Delta x,\ y = j\Delta y,\ z = k\Delta z.$ $\Delta x = \Delta y = \Delta z$

we will use this form

$$V(i, j, k) \equiv V(i\Delta x, j\Delta y, k\Delta z)$$

$$\frac{\partial V}{\partial x} \approx \frac{V(i+1, j, k) - V(i, j, k)}{\Delta x}$$

Eq. (5.2)

or

$$\frac{\partial V}{\partial x} \approx \frac{V(i+1, j, k) - V(i-1, j, k)}{2\,\Delta x}$$

$$\frac{\partial V}{\partial x} \approx \frac{V(i, j, k) - V(i-1, j, k)}{\Delta x}$$

"best" choice depends on the particular problem at hand.

Discretisation

the derivatives are to be evaluated at the locations $(i \pm \frac{1}{2})$

$$\frac{\partial^2 V}{\partial x^2} \approx \frac{1}{\Delta x}\left[\frac{\partial V}{\partial x}(i + \tfrac{1}{2}) - \frac{\partial V}{\partial x}(i - \tfrac{1}{2})\right]$$

$$\frac{\partial^2 V}{\partial x^2} \approx \frac{1}{\Delta x}\left[\frac{V(i+1, j, k) - V(i, j, k)}{\Delta x} - \frac{V(i, j, k) - V(i-1, j, k)}{\Delta x}\right]$$

$$= \frac{V(i+1, j, k) + V(i-1, j, k) - 2\,V(i, j, k)}{(\Delta x)^2}$$

Eq. (5.7)

Inserting them all into Laplace's equation and solving for $V(i, j, k)$

$$V(i, j, k) = \frac{1}{6}\,[V(i+1, j, k) + V(i-1, j, k) + V(i, j+1, k) + V(i, j-1, k) + V(i, j, k+1) + V(i, j, k-1)]$$

Eq. (5.8)

Jacobi method of relaxation

- To evaluate the value of V at each point (i,j,k) according to Eq. (5.8), we assume that the boundary conditions: values of V at the boundary: $V(-1,0,0)$, $V(1,0,0)$, $V(0,-1,0)$, $V(0,1,0)$, $V(0,0,-1)$, $V(0,0,1)$, are known.
- Then we put forward an initial guess of $V(i,j,k)$ for each (i,j,k), call it $V_0(i,j,k)$. Insert this initial profile to the RHS of Eq. (5.8) to work out an “improved” profile $V_1(i,j,k)$. Then $V_1(i,j,k)$ is in turn inserted into the RHS of Eq. (5.8) again.

$$V(i,j,k) = \frac{1}{6}\left[V(i+1,j,k) + V(i-1,j,k) + V(i,j+1,k) + V(i,j-1,k) + V(i,j,k+1) + V(i,j,k-1)\right] \qquad \text{Eq. (5.8)}$$

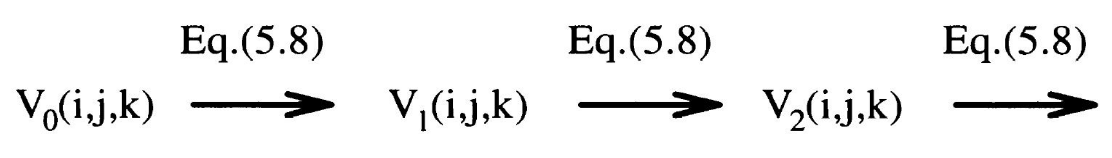


Figure 5.1: Schematic flowchart for the relaxation algorithm.

Jacobi method of relaxation

- In each iteration the solution $V_n\,(i,j,k)$ "relaxes" to a more presumably "correct" values $V_{n+1}\,(i,j,k)$.
- The relaxation is continued until a satisfying convergence requirement is achieved for the V profile,
- $(1/N)\sum_{\{i,j\}}[V_{n+1}(i,j,k) - V_n(i,j,k)]^2 = \Delta V_n <$ tol, for all (i,j,k). N = total number of grid points = $i_{\max} \times j_{\max}$
- In practice, we monitor ΔV_n in each iteration n. Solution for $V_n(i,j,k)$ is said to be achieved once $\Delta V_n <$ tol, where tol a convergence criteria set by us.

Implementation of Jacobi relaxation method for Laplace equation in 2-D

- For a 2-D case, $V = V(i,j)$

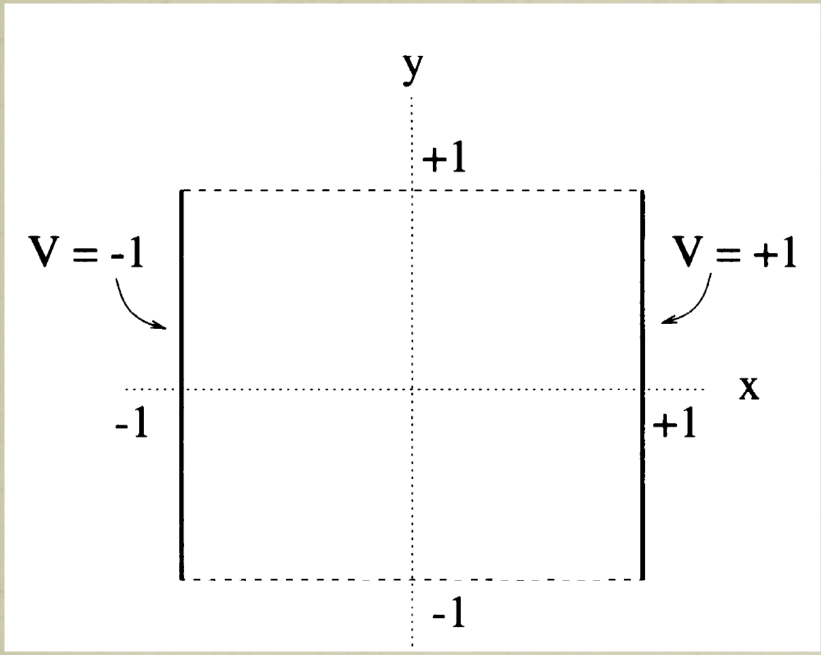
$$\frac{\partial^2 \mathbf{V}(\mathbf{x},\mathbf{y})}{\partial^2 \mathbf{x}} + \frac{\partial^2 \mathbf{V}(\mathbf{x},\mathbf{y})}{\partial^2 \mathbf{y}} = 0$$

$$V_{n+1} = \frac{1}{4}\left[V_n\left(i+1,\, j\right)+V_n\left(i-1,\, j\right)+V_n\left(i,\, j+1\right)+V_n\left(i,\, j-1\right)\right]$$

or

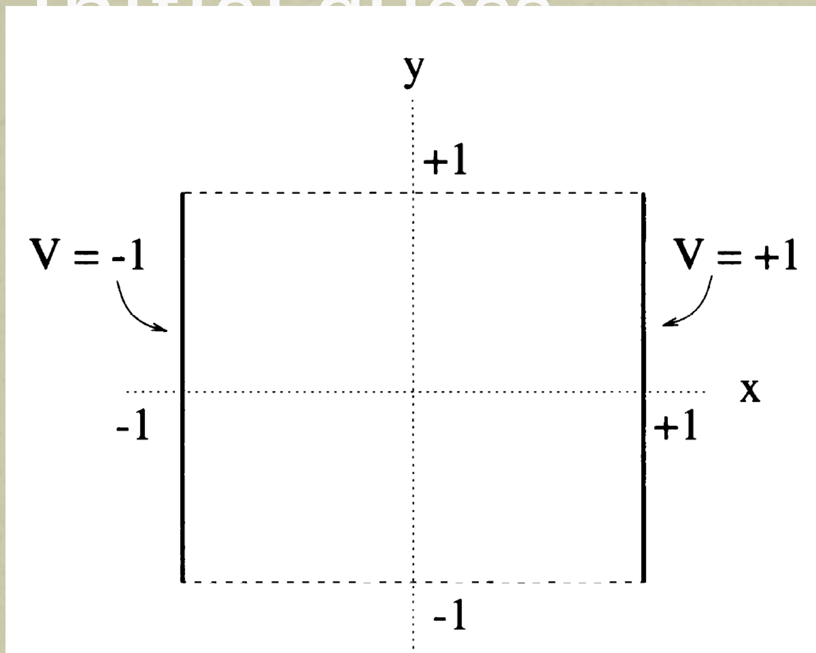
$$V_{\text{new}} = \frac{1}{4}\left[V_{\text{old}}\left(i+1,\, j\right)+V_{\text{old}}\left(i-1,\, j\right)+V_{\text{old}}\left(i,\, j+1\right)+V_{\text{old}}\left(i,\, j-1\right)\right]$$

Implementation on a 2-D plate (infinite extent)

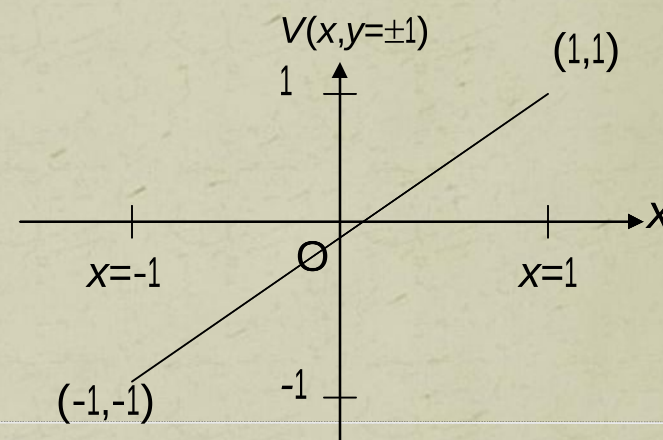


- Boundary condition:
- $V(-1,j)=-1$; $V(1,j)=1$;
- Range of coordinates:
- $x_{i=0}=-1.0$;
- $x_{i+1}=x_i+\Delta x$;
- $x_{i=N} = 1.0$;
- $\Delta x = (x_{i=N} - x_{i=0})/N$
- Similarly for *y*-component.
- *N* is the “resolution” of your simulation.

Initial guess



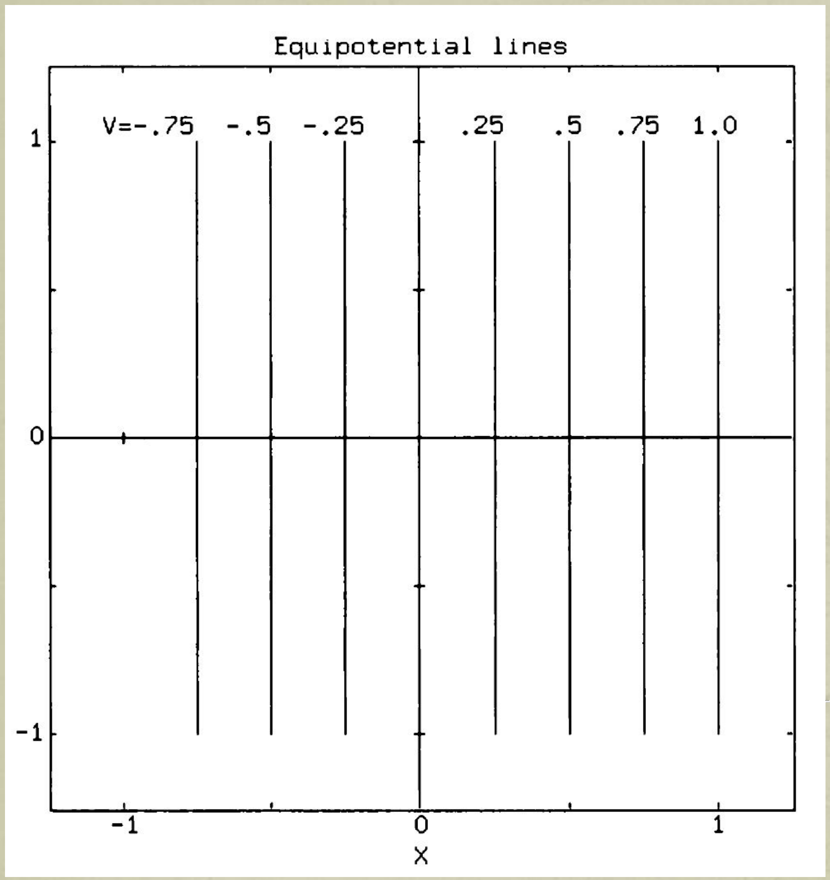
$$V(x,y)=\begin{cases} x\times \text{gradient -1}, x\in[0,1], y=\pm 1 \\ 1, x=\pm 1, y\in[0,1] \\ 0, \text{else} \end{cases}$$



Initial guess: V_0 N=6

-1.00	-.67	-.33	.00	.33	.67	1.00
-1.00	.00	.00	.00	.00	.00	1.00
-1.00	.00	.00	.00	.00	.00	1.00
-1.00	.00	.00	.00	.00	.00	1.00
-1.00	.00	.00	.00	.00	.00	1.00
-1.00	.00	.00	.00	.00	.00	1.00
-1.00	-.67	-.33	.00	.33	.67	1.00

Output



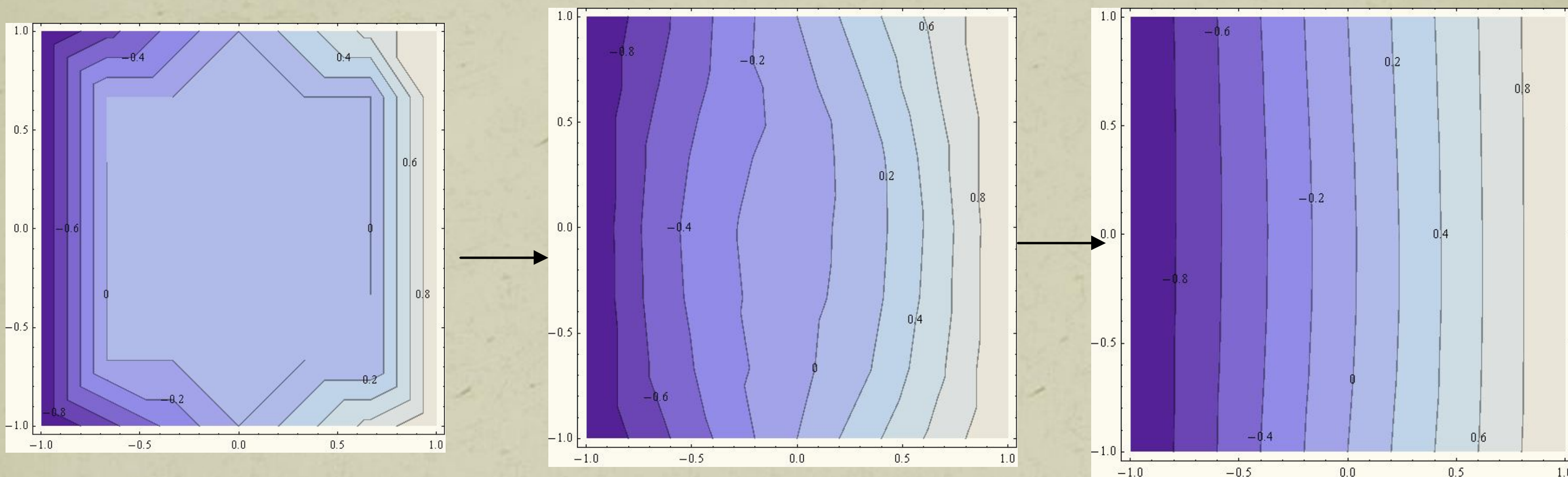
- The output is a list of $V(i,j)$ for all position (i,j).
- Equipotential lines are to be plotted on the *x*-*y* plane. These equipotentials shall appear stationary on the xy plane when convergence is acchieved.
- A Mathematica code has to be developed to plot the equipotential lines based on $V(i,j)$ generated.

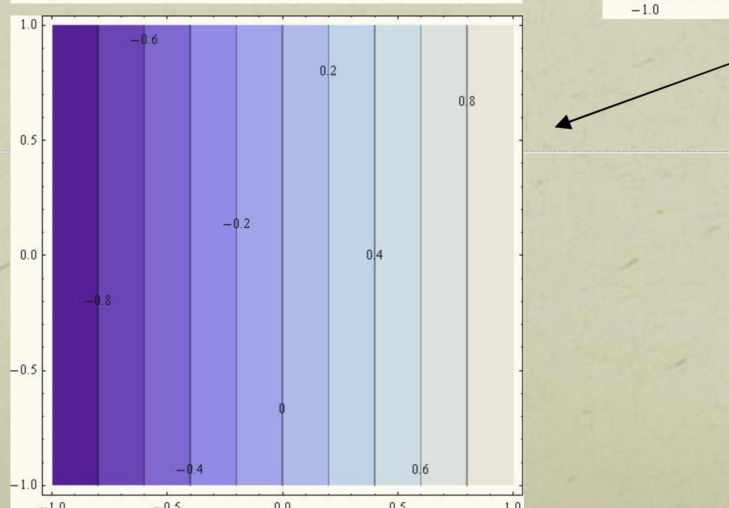
Program structure

- Call a subroutine to generate an initial trial potential profile $V(i,j)$.
- Iterate
  - Call the update program-V subroutine to update V_{n+1} based on V_n
  - Check ΔV_n
  - Display $V_n(i,j)$ to monitor the variation visually (via movie)
  - Break if $\Delta V_n < tol$
- Mathematica's powerful displaying capability is good for such purpose.

2D Contour Plot of equipotential

The final results for the potential are plotted as equipotential contours[6]





ListContourPlot
or
ListDensityPlot

Electric field

For generic 3D case,

$\mathbf{E} = \mathbf{E}(x,y,z) = \mathbf{E}_x(x,y) + \mathbf{E}_y(x,y) + \mathbf{E}_z(x,y)$

$\mathbf{E} = -\nabla V(x,y,z)$

$$= -\frac{\partial \boldsymbol{V}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}{\partial \boldsymbol{x}}\mathbf{i} - \frac{\partial \boldsymbol{V}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}{\partial \boldsymbol{y}}\mathbf{j} - \frac{\partial \boldsymbol{V}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{z})}{\partial \boldsymbol{z}}\mathbf{k}$$

For a 2D case, $E=E(x,y)$ only:

$\mathbf{E} = \mathbf{E}_x(x,y) + \mathbf{E}_y(x,y)$

Electric field

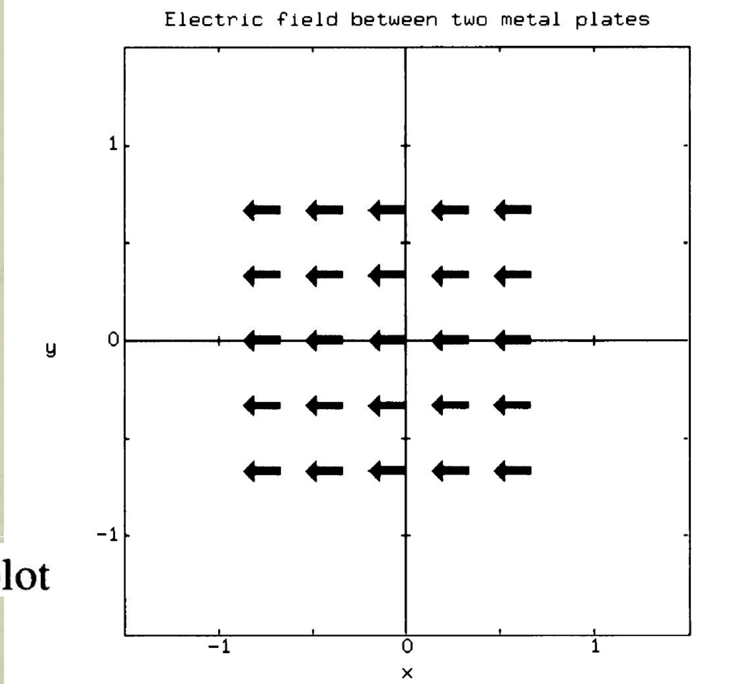
These results for V can be used to obtain the electric field

$$E_x = -\frac{\partial V}{\partial x}$$

$$E_x(i,j) \approx -\frac{V(i+1,j) - V(i-1,j)}{2\,\Delta x}$$

with corresponding relations for E_y and E_z.

vector plot



Here each arrow is oriented in the direction of $\vec{E}$ at that location, and the length of each arrow is proportional to the magnitude of the field.

Hollow metallic prism with a solid inner conductor

- This is your homework assignment.

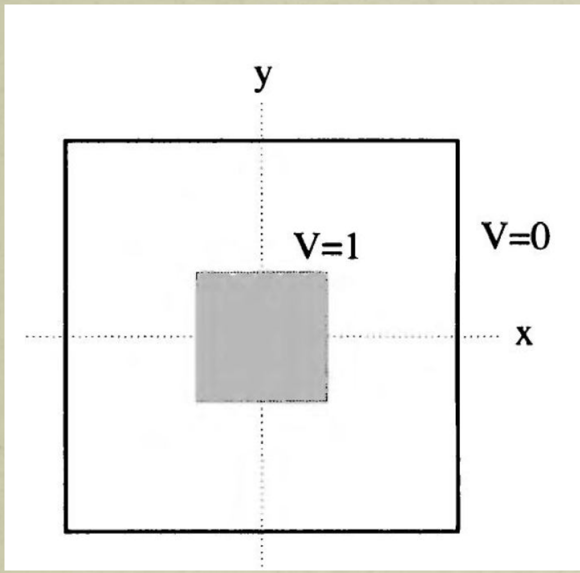


Figure 5.4: Schematic cross section of a hollow metallic prism with a solid, metallic inner conductor. The prism and inner conductor are presumed to be infinite in extent along z. The inner conductor is held at $V = 1$ and the walls of the prism at $V = 0$.

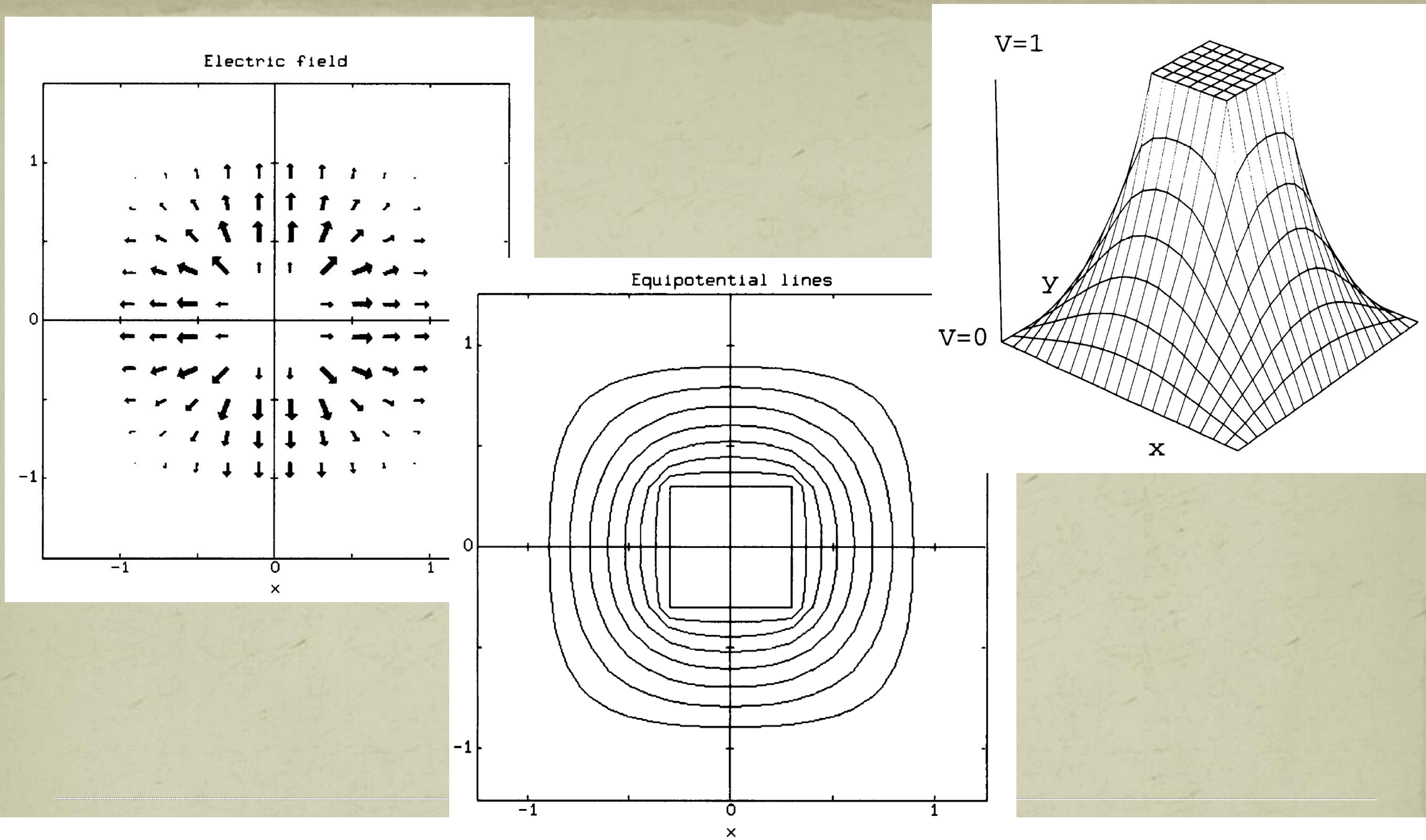


Figure 5.5: Electric potential and field inside the prism in Figure 5.4. The sides of the prism in the x–y plane had lengths of 2 units, and the inner conductor had an edge length of 0.6 units. The spatial grid size was 0.1. Upper left: equipotential contours; upper right: perspective plot of the potential; bottom: electric field.

Potentials and Fields Near electric charge

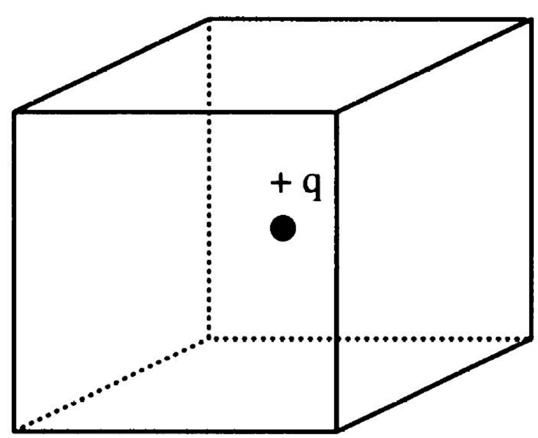
$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{\rho}{\epsilon_0},$$

Poisson's equation,

$$V(i,j,k) = \frac{1}{6}[V(i+1,j,k) + V(i-1,j,k) + V(i,j+1,k) + V(i,j-1,k) + V(i,j,k+1) + V(i,j,k-1)] + \frac{\rho(i,j,k)\,(\Delta x)^2}{6\,\epsilon_0}, \qquad (5.17)$$

Make sure you know how to derive this difference equation!!

a single-point charge in three dimensions.



$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} + \frac{\partial^2 V}{\partial z^2} = -\frac{\rho}{\epsilon_0},$$

$$\texttt{rho(0, 0, 0)} = q/\mathrm{dx}^3$$

Figure 5.8: Schematic of a point charge $+q$ located at the center of a metal box. The faces of the box are all held at $V = 0$.

Metal box: potential at the walls vanishes.

a single-point charge in three dimensions.

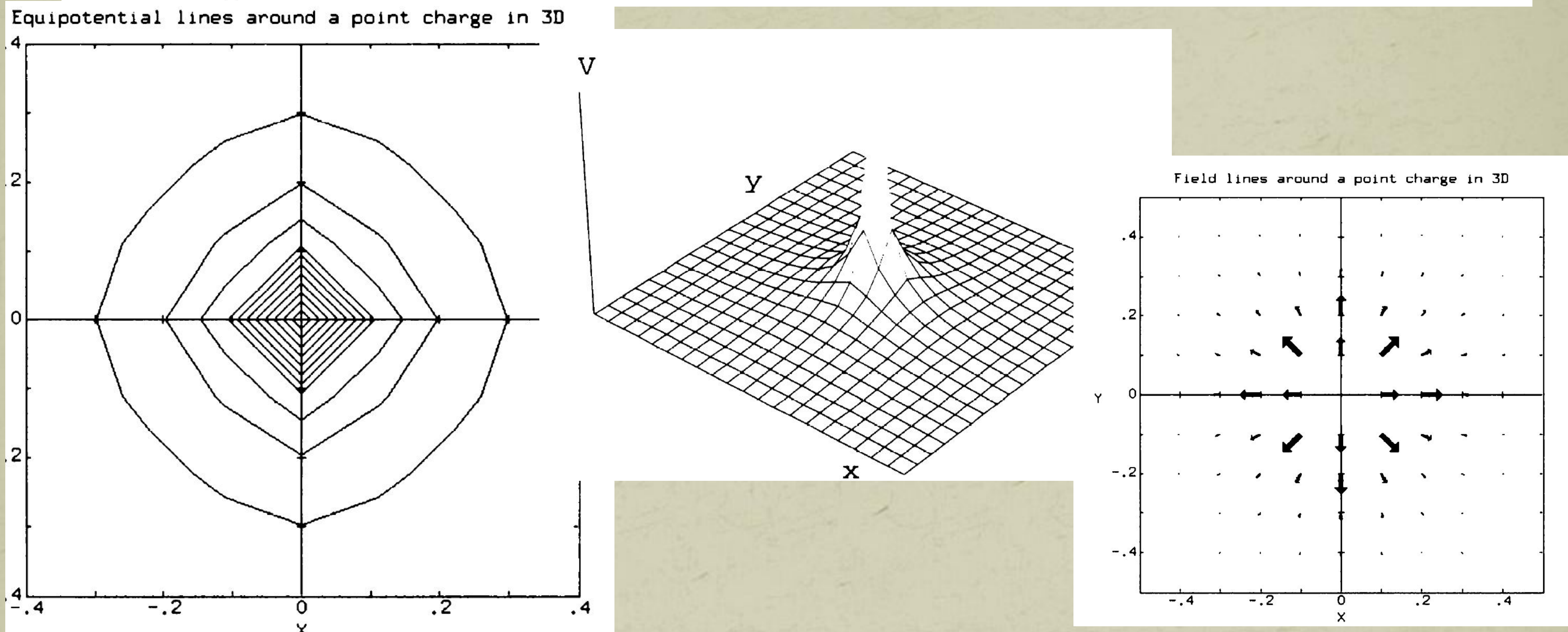


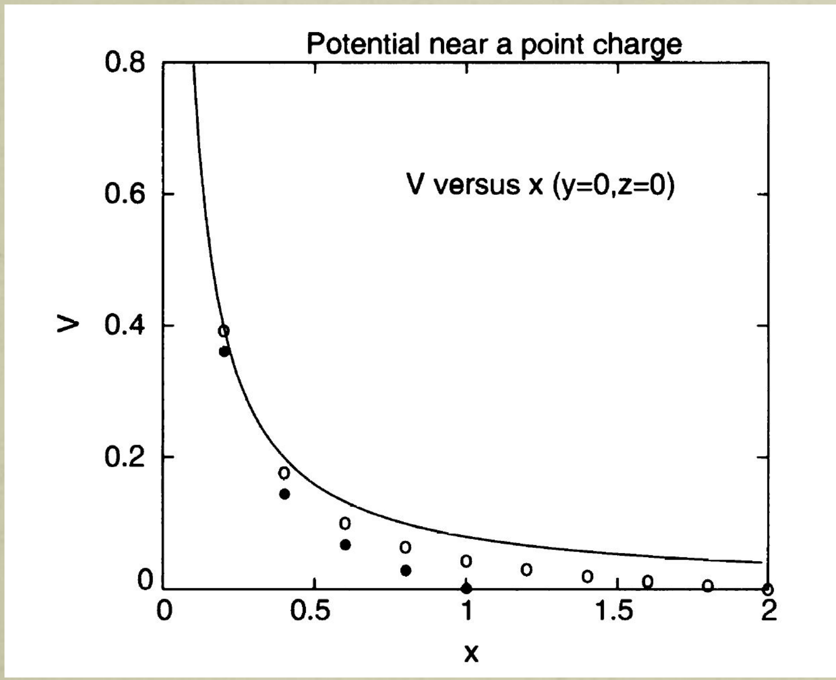
Figure 5.9: Results for the electric potential and field near a point charge located at the center of a metal box. The box had an edge length of 2 (x, y, and z all ran from -1 to $+1$) and the spatial step size was 0.1. Upper left: equipotential lines; upper right: perspective plot of the potential in the $z = 0$ plane; bottom: electric field (note that the length of each arrow is proportional to the field strength at the point where the base of the arrow is located). Also note that the arrows closest to the origin are "distorted"; the singularity at the origin together with the finite difference expression used to compute E makes the value smaller than it should ideally be. The plots on the upper left and right show only the potential and field near the center of the box.

Code

- Generalise the 2D Laplace Equation to 3D Poisson equation. Use the Jacobi relaxation method to solve the point charge in the box problem.
- Visualise the potential and electric vectorial fields using ListDensityPlot (or ListContourPlot) and ListPlotVector, ListPlotVector3D.

a single-point charge in three dimensions.

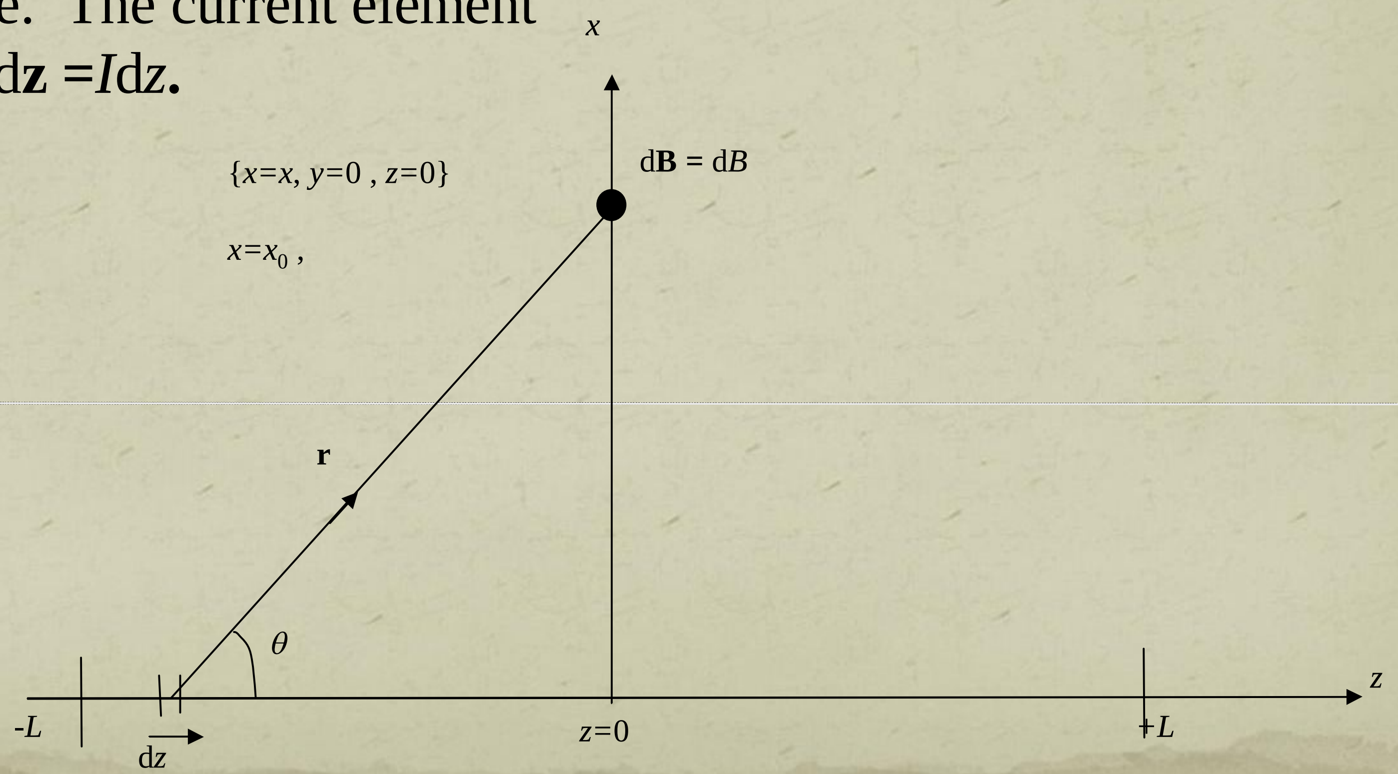
$$V(r) = \frac{q}{4\pi\epsilon_0 r},$$



- Compare your numerical solution with the Coulomb law, which is the solution to Poisson equation for the simple point charge in a large 3D box.
- In the simulation, the numerical solution improve (compares better to the analytical one) as the size of the simulation box gets larger (which in turn consumes more expansive computational resource.)

5.3 Magnetic field produced by a current – simplest case

- Wire of length 2*L*. Current *I* is to flow from left to right. The magnetic field is perpendicular to and directed inwards to the x-z plane. The current element is d**I** = *I*d**z** =*I*dz**.**



Vectors

- Vector notation: $\hat{i} \equiv \hat{x}; \hat{j} \equiv \hat{y}; \hat{k} \equiv \hat{z}$

- Reminder for vectors: cyclic permutation and right hand rule, e.g.,

$$\hat{i} \times \hat{j} = \hat{k}; \hat{k} \times \hat{i} = \hat{j}; \hat{j} \times \hat{i} = -\hat{k}, ...; \hat{i} \times \hat{i} = \hat{j} \times \hat{j} = \hat{k} \times \hat{k} = 0$$

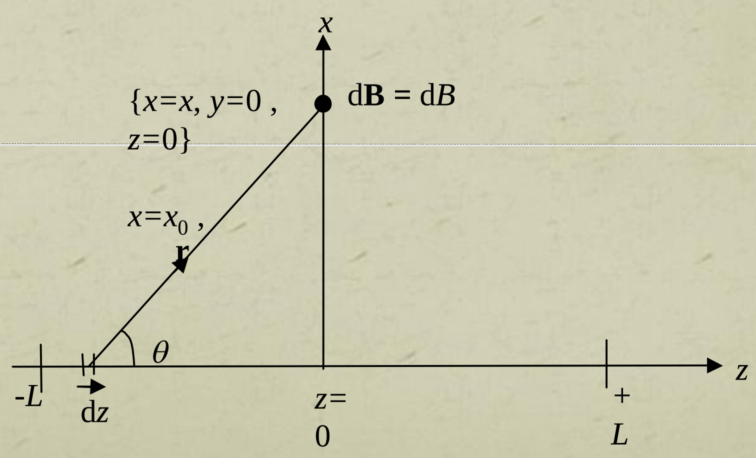
Bior-Savart law for magnetic field

- Bior-Savart law for magnetic field at the fixed point {x=x, y=0 , z=0}, produced by a current element $d\mathbf{I}$ is

$$d\mathbf{B} = \frac{\mu_0}{4\pi}\frac{d\mathbf{I}\times\hat{r}}{r^2} = \frac{\mu_0 I dz}{4\pi r^2}\hat{k}\times\hat{r} = \frac{\mu_0}{4\pi}\frac{d\mathbf{I}\times r\hat{r}}{r^3} = \frac{\mu_0}{4\pi}\frac{d\mathbf{I}\times\mathbf{r}}{r^3} = \frac{\mu_0 I dz}{4\pi r^3}\hat{k}\times\mathbf{r}$$

Since $\hat{k}\times\hat{r} = \hat{k}\times\left(\hat{i}\sin\theta + \hat{k}\cos\theta\right) = \hat{k}\times\hat{i}\sin\theta = \hat{j}\sin\theta$

$$d\mathbf{B} = \frac{\mu_0 I dz}{4\pi r^2}\sin\theta\,\hat{j} = d\mathbf{B}_y$$



Discretising Bior-Savart formula

- Using simple geometry, $\dfrac{\sin\theta}{r^2} = \dfrac{x/r}{z^2+x^2} = \dfrac{x/\sqrt{z^2+x^2}}{z^2+x^2} = \dfrac{x}{\left(z^2+x^2\right)^{3/2}}$

- Hence $d\mathbf{B} = \dfrac{\mu_0 I \mathrm{dz}}{4\pi} \dfrac{x}{\left(z^2+x^2\right)^{3/2}} \hat{j} \Rightarrow dB = \dfrac{\mu_0 I}{4\pi} \dfrac{x}{\left(z^2+x^2\right)^{3/2}} \mathrm{dz}$

- Discretising, $\Delta B(x) = \dfrac{\mu_0 I}{4\pi} \dfrac{x}{\left(z^2+x^2\right)^{3/2}} \Delta z$
- The total magnetic field is obtained by summing over all contribution from element Δz

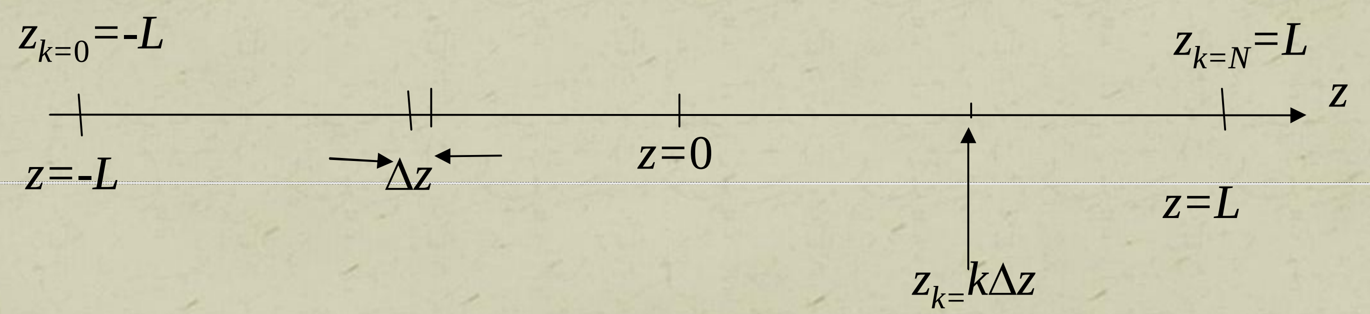
$$B(x) = \sum_{\text{all } \Delta z \text{ along } z} \frac{\mu_0 I}{4\pi} \frac{x}{\left(z^2+x^2\right)^{3/2}} \Delta z \qquad \text{(Eq. 5.25)}$$

Partitioning of the z-axis

- This sum can be evaluated numerically via (x is fixed)

$$\sum_{\text{all } \Delta z \text{ along } z} \frac{\mu_0 I}{4\pi} \frac{x}{\left(z^2 + x^2\right)^{3/2}} \Delta z = \sum_{\text{all } k} \frac{\mu_0 I}{4\pi} \frac{x}{\left(z_k{}^2 + x^2\right)^{3/2}} \Delta z = \frac{\mu_0 I}{4\pi} \sum_k \frac{x}{\left(\left(k\Delta z\right)^2 + x^2\right)^{3/2}} \Delta z;$$

$$z_k = k\Delta z$$



Pseudocode

- Pseudocode:
- Choose the size of the simulation "box", $[-L, L]$.
- Then choose the size of the interval, Δz.
- The number of intervals NStep is determined by $2L/\Delta z$.
- $z[0] = -L$; $z[\text{NStep}] = L$;
- $z[k] = z[0] + k\,\Delta z$, $k \in [1,\text{Nstep}]$;
- Then sum over all k to obtain Eq.(5.25)
- Repeat for next value of x.

At the end, B as a function of x would be obtained.

Analytical solution

- The analytical solution for the Biot-Savart law for an infinite current carrying wire is given by

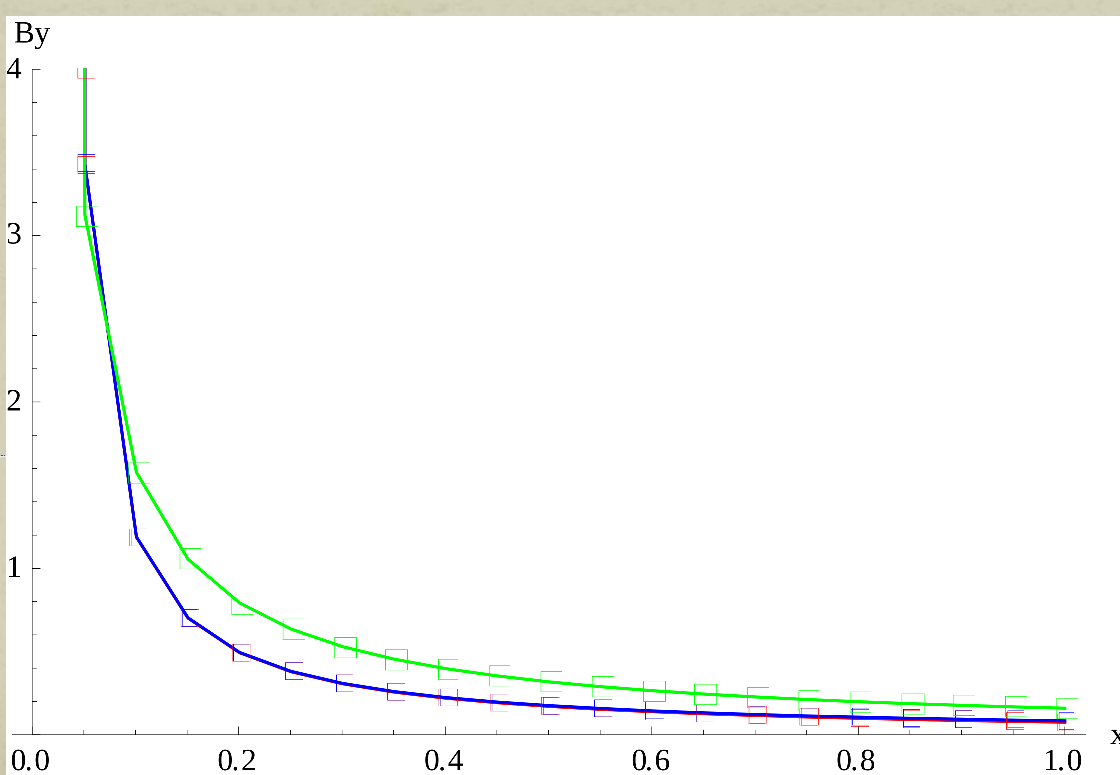
$$B(x) = \frac{\mu_0 I}{2\pi x}$$

- We can compare the numerical answer Eq. (5.25) with it.

- The numerical sum Eq. (5.25) for longer wire behaves closer to the analytical one. In addition, the discretisation effect sets in when $x \rightarrow \Delta z$. In this limit large error shows up.

Numerical vs. analytical solution

- The values based on Eq. (5.25), and analytical solution are plotted for x=(0,1.0], *L*=1 (Red), *L*=10 (Blue), and Green (analytical), using Mathematica code.



Trapezoid rule for integration

- Note that the sum $\sum_k \frac{\mu_0 I}{4\pi} \frac{x_0}{\left(z_k^{\ 2} + x_0^{\ 2}\right)^{3/2}} \Delta z \equiv \sum_k f\left(z_k\right) \Delta z$

approximates the integral $\int f(z)dz$

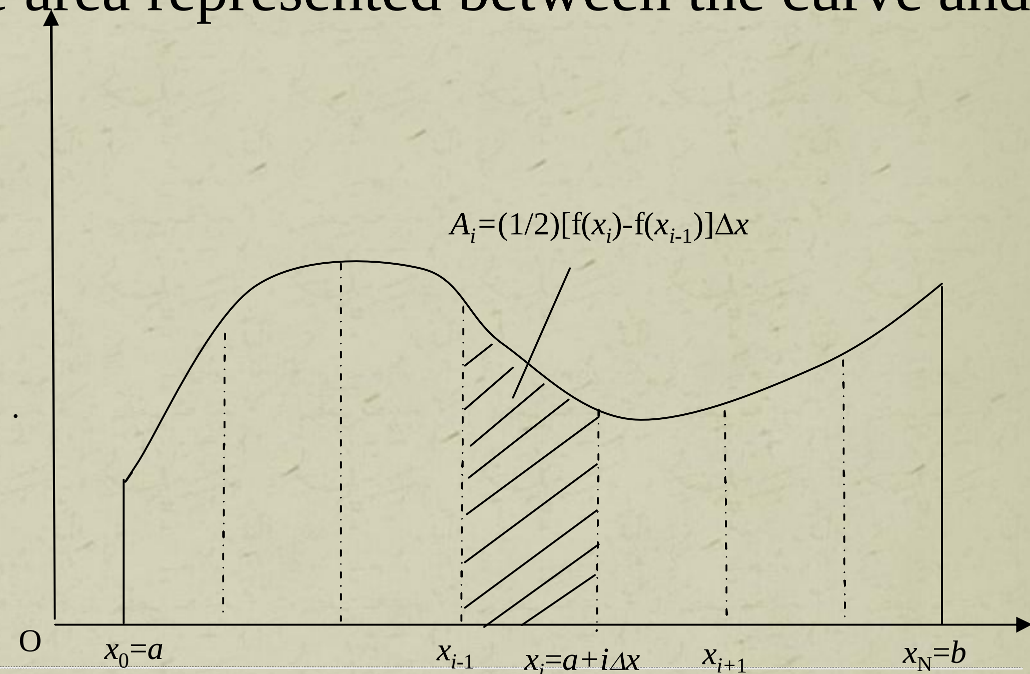
Many methods can be used to numerically evaluate the integral

$\int f(z)dz$

Basically the integral is the area represented between the curve and the vertical axis.

Trapezoid rule for integration

Basically the integral is the area represented between the curve and the x-axis.



Trapezoidal rule:

$$\int f(x)dx \approx \sum_{i=0}^{i=N} A_i = \sum_{i=0}^{i=N} \frac{1}{2}\Delta x\left[f(x_{i+1}) + f(x_i)\right]$$

$$= \Delta x \cdot \left\{\frac{1}{2}\left[f(x_0) + f(x_1)\right] + \frac{1}{2}\left[f(x_1) + f(x_2)\right] + \cdots + \frac{1}{2}\left[f(x_{N-2}) + f(x_{N-1})\right] + \frac{1}{2}\left[f(x_{N-1}) + f(x_N)\right]\right\}$$

$$= \frac{\Delta x}{2}\left[f(x_0) + f(x_N)\right] + \Delta x\left[f(x_1) + f(x_2) + \cdots + f(x_{N-2}) + f(x_{N-1})\right]$$

$$= \frac{\Delta x}{2}\left[f(x_0) + f(x_N)\right] + \sum_{i=1}^{i=N-1} f(x_i)$$

The error, is of the order $O(\Delta x)^2$

Simpson's rule for integration

- The numerical integration can be improved by treating the curve connecting the point $\{x_{i+1}, f(x_{i+1})\}, \{x_i, f(x_i)\}$ as a section of a parabola instead of a straight line (as was assumed in trapezoid rule).
- This results in $A_i + A_{i+1} = (\Delta x/3)[f(x_i) + f(x_{i+1}) + f(x_{i+2})]$.
- Hence,

$$\int_a^b f(x)dx \approx \sum_{0,2,4,\ldots,N-2} A_i + A_{i+1} = \frac{\Delta x}{3} \sum_{0,2,4,\ldots,N-2} f(x_i) + 4f(x_{i+1}) + f(x_{i+2})$$

$$= \frac{\Delta x}{3}\begin{pmatrix} \left[f(x_0)+4f(x_{0+1})+f(x_{0+2})\right]+\left[f(x_2)+4f(x_{2+1})+f(x_{2+2})\right]+\left[f(x_4)+4f(x_{4+1})+f(x_{4+2})\right]+\cdots \\ +\left[f(x_{N-2})+4f(x_{N-1})+f(x_N)\right] \end{pmatrix}$$

$$= \frac{\Delta x}{3}\left\{f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+4f(x_5)+2f(x_6)+\cdots+2f(x_{N-2})+4f(x_{N-1})+f(x_N)\right\}$$

with error of $O(\Delta x)^4$

Simpson's rule for integration

- For our purpose, we are to evaluate the integration

$$\int f(z)dz \approx \sum_k A_k = \sum_k f(z_k)\Delta z \qquad \text{Eq. (5.26)} \quad \text{where}$$

$$f(z) \equiv \frac{\mu_0 I}{4\pi}\frac{x}{\left(z^2+x^2\right)^{3/2}}$$

Simpson's rule:

$$\int_a^b f(x)dx \approx \frac{\Delta x}{3}\left[f(a)+f(b)\right]+\frac{4\Delta x}{3}\left[f(x_1)+f(x_3)+f(x_5)+\cdots f(x_N)\right]$$

$$+\frac{2\Delta x}{3}\left[f(x_2)+f(x_4)+f(x_6)+\cdots f(x_N-1)\right]$$

Here, *N* has to be an large odd number. The number of interval, *N*, matters: if it is too small, large error occurs. Choose *N* = 101 is sufficient.