shooting method example

✔ the equation modeling the temperature y of a heat transfer pipe at distance x is:

$$\boxed{\frac{d^2y}{dx^2} = 2y} \qquad \begin{cases} y(x=0) & = & 1 \\ y'(x=1) & = & 0 \end{cases}$$

✔ analytic solution:

$$\boxed{y(x) = a_1 e^{\sqrt{2}x} + a_1 e^{-\sqrt{2}x}} \qquad \begin{vmatrix} a_1 = 0.05581 \\ a_2 = 0.94419 \end{vmatrix}$$

✔ shooting method

transform 2nd-order into a 1st-order system

$$\begin{cases} \frac{dy}{dx} = z \\ \frac{dz}{dx} = 2y \end{cases} \qquad \begin{vmatrix} y(0) = 1 \\ z(1) = 0 \end{vmatrix}$$

✔ transform to an initial value problem with a trial hypothesis to start $\mathbf{u}$

$$\begin{cases} y(0) = 1 \\ z(0) = u \end{cases}$$

✔ iterate equation solutions with RK4 method through all the $\mathbf{x}$ interval and retrieve the value for $\mathbf{z}$ function at the boundary

$$z_{iter}(1) \equiv g(u)$$

✔ solve the following equation in order to find the right initial value providing the boundary condition $\mathbf{z(1) = 0}$

$$z(1) - g(u) = 0$$

root finding algorithm will provide iterated $\mathbf{u_i}$'s for introducing on RK4

shooting method example

✔ first iteration on root finding (RK4)

$y(0) = 1, z(0) = 0$

x	y	z
0	1	0
0.2	1.04027	0.405333
0.4	1.1643	0.84331
0.6	1.3821	1.3492
0.8	1.71119	1.96373
1	2.17807	2.73641

✔ second iteration on root finding (RK4)

$y(0) = 1, z(0) = -2$

x	y	z
0	1	-2
0.2	0.634933	-1.6752
0.4	0.320993	-1.4853
0.6	0.0328983	-1.41499
0.8	-0.252549	-1.45864
1	-0.558335	-1.61974

✔ secant method: find next initial value iteration

$$\begin{cases} u_0 = 0 & g(0) = 2.73641 \\ u_1 = -2 & g(-2) = -1.61974 \end{cases}$$

$$u_2 = u_1 - g(u_1)\frac{u_1 - u_0}{g(u_1) - g(u_0)}$$

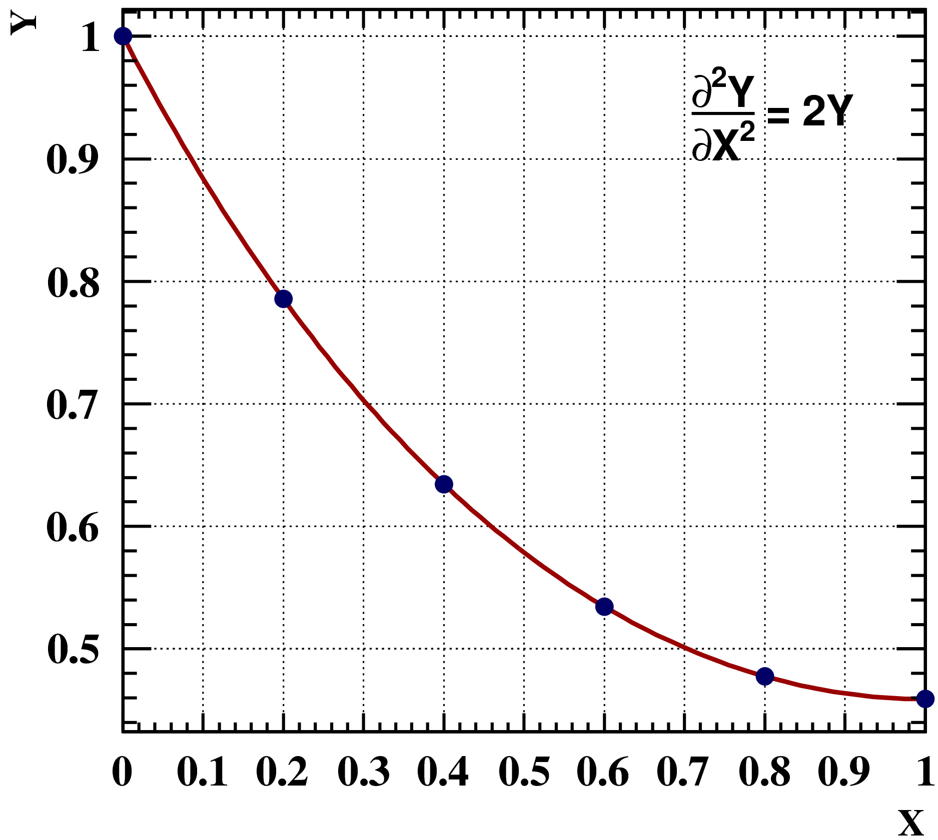
$$= -2 + 1.62 \frac{-2-0}{-1.62 - -2.736} = -1.256$$

✔ third iteration on root finding (RK4)

$y(0) = 1, z(0) = -1.256$

x	y	z
0	1	-1.25634
0.2	0.785648	-0.901599
0.4	0.634559	-0.619454
0.6	0.534568	-0.38719
0.8	0.477623	-0.186103
1	0.459138	3.05311e − 16

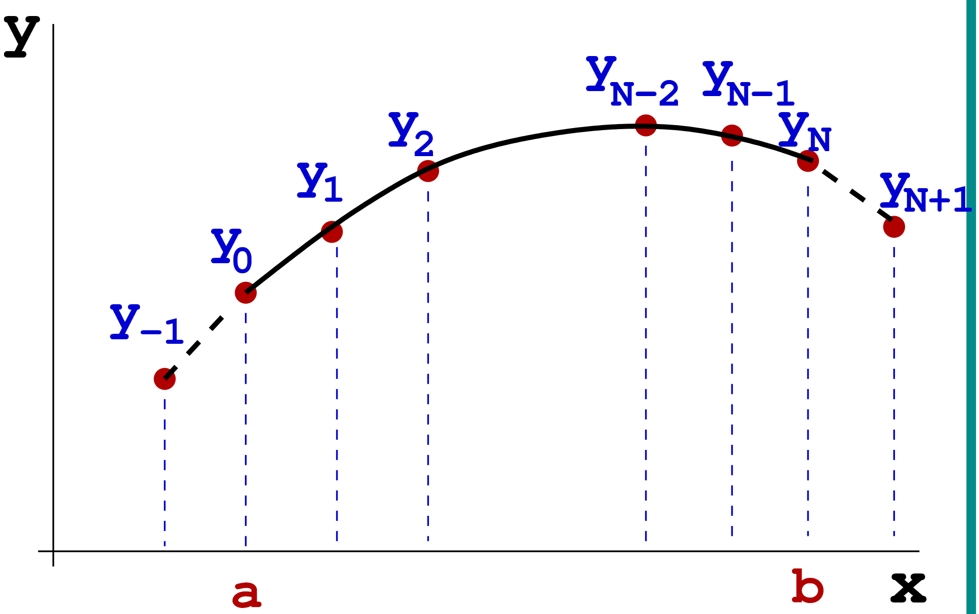
shooting method: solution



BV problems: finite-differences

In the finite-difference method, the independent variable (x) is discretized and we transform the differential equation into a set of algebraic equations

the purpose of the equation system is to find the function value at every mesh point



BV problems: finite-differences

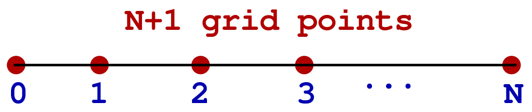
- ✔ discretize the interval $x \in [a,b]$ in $N+1$ grid points: $k = 0, \cdots, N$

  grid spacing $h = \frac{b-a}{N}$

- ✔ using the central difference derivative at the grid points

$$y''(x_k) \equiv y''_k = \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2}$$

$$y'(x_k) \equiv y'_k = \frac{y_{k+1} - y_{k-1}}{2h}$$



- ✔ the differential equation becomes for the inner grid points $k = 1, \cdots, N-1$

$$a(x)\, y''(x) + b(x)\, y'(x) + c(x)\, y(x) = f(x)$$

$$a_k \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} + b_k \frac{y_{k+1} - y_{k-1}}{2h} + c_k y_k = f_k$$

sorting the y_k terms, we define a set of linear equations:

$$\boxed{\left(\frac{a_k}{h^2} - \frac{b_k}{2h}\right) y_{k-1} + \left(c_k - 2\frac{a_k}{h^2}\right) y_k + \left(\frac{a_k}{h^2} + \frac{b_k}{2h}\right) y_{k+1} = f_k} \qquad k = 1, \cdots, N-1$$

BV problems: finite-differences (cont.)

- ✔ the boundary problem reduces to a system of linear equations at the inner mesh points:

$$\begin{cases}
\left(\frac{a_1}{h^2} - \frac{b_1}{2h}\right) y_0 & + \left(c_1 - 2\frac{a_1}{h^2}\right) y_1 & + \left(\frac{a_1}{h^2} + \frac{b_1}{2h}\right) y_2 & = f_1 & \text{(k=1)} \\
\left(\frac{a_2}{h^2} - \frac{b_2}{2h}\right) y_1 & + \left(c_2 - 2\frac{a_2}{h^2}\right) y_2 & + \left(\frac{a_2}{h^2} + \frac{b_2}{2h}\right) y_3 & = f_2 & \text{(k=2)} \\
\cdots & + \cdots & + \cdots & = \cdots & \\
\left(\frac{a_{N-1}}{h^2} - \frac{b_{N-1}}{2h}\right) y_{N-2} & + \left(c_3 - 2\frac{a_{N-1}}{h^2}\right) y_{N-1} & + \left(\frac{a_{N-1}}{h^2} + \frac{b_{N-1}}{2h}\right) y_N & = f_{N-1} & \text{(k=N-1)}
\end{cases}$$

The boundary conditions:

$$\begin{cases} y(a) = \lambda_1 & \text{or} & y'(a) = \lambda_1 \\ y(b) = \lambda_2 & \text{or} & y'(b) = \lambda_2 \end{cases}$$

The boundary conditions approximating the derivatives:

$$\begin{cases} y(a) = \lambda_1 & \text{or} & \frac{y_1 - y_{-1}}{2h} = \lambda_1 \\ y(b) = \lambda_2 & \text{or} & \frac{y_{N+1} - y_{N-1}}{2h} = \lambda_2 \end{cases}$$

BV problems: finite-differences (cont.)

- Two additional equations are added at the extreme mesh points:
  - either we know immediately the solutions $\mathbf{y_0}$ and $\mathbf{y_N}$ from the boundary conditions, and the two equations are:

$$y_0 = \lambda_1$$
$$y_N = \lambda_2$$

  - or if the boundary conditions are derivatives, we introduce new equations at the extreme mesh points,

$$(k=0) \quad \left(\frac{a_0}{h^2} - \frac{b_0}{2h}\right) y_{-1} + \left(c_0 - 2\frac{a_0}{h^2}\right) y_0 + \left(\frac{a_0}{h^2} + \frac{b_0}{2h}\right) y_1 = f_0$$
$$(k=N) \quad \left(\frac{a_N}{h^2} - \frac{b_N}{2h}\right) y_{N-1} + \left(c_N - 2\frac{a_N}{h^2}\right) y_N + \left(\frac{a_N}{h^2} + \frac{b_N}{2h}\right) y_{N+1} = f_N$$

The additional mesh points $\mathbf{y_{-1}}$ and $\mathbf{y_{N+1}}$ outside the equation range $[\mathbf{a}, \mathbf{b}]$ can be eliminated from the boundary conditions,

$$(k=0) \quad \left(\frac{a_0}{h^2} - \frac{b_0}{2h}\right)(y_1 - 2h\lambda_1) + \left(c_0 - 2\frac{a_0}{h^2}\right) y_0 + \left(\frac{a_0}{h^2} + \frac{b_0}{2h}\right) y_1 = f_0$$
$$\left(c_0 - 2\frac{a_0}{h^2}\right) y_0 + \left(2\frac{a_0}{h^2}\right) y_1 = f_0 + 2h\lambda_1\left(\frac{a_0}{h^2} - \frac{b_0}{2h}\right)$$

$$(k=N) \quad \left(\frac{a_N}{h^2} - \frac{b_N}{2h}\right) y_{N-1} + \left(c_N - 2\frac{a_N}{h^2}\right) y_N + \left(\frac{a_N}{h^2} + \frac{b_N}{2h}\right)(y_{N-1} + 2h\lambda_2) = f_N$$
$$\left(2\frac{a_N}{h^2}\right) y_{N-1} + \left(c_N - 2\frac{a_N}{h^2}\right) y_N = f_N - 2h\lambda_2\left(\frac{a_N}{h^2} - \frac{b_N}{2h}\right)$$

finite-difference method example

- the equation modelling the temperature y of a heat transfer pipe at distance x is:

$$\boxed{\frac{d^2y}{dx^2} = 2y} \qquad \begin{cases} y(x=0) = 1 \\ y'(x=1) = 0 \end{cases}$$

- analytic solution:

$$\boxed{y(x) = a_1 e^{\sqrt{2}x} + a_1 e^{-\sqrt{2}x}} \qquad a_1 = 0.05581, \quad a_2 = 0.94419$$

- finite-difference method

  discretize $\mathbf{x}$ variable in the range where we want to solve the differential equation $[\mathbf{0}, \mathbf{1}]$

  using a step $\mathbf{h = 0.1}$, the range is divided in $\mathbf{10}$ sub-intervals and the grid points are $\mathbf{x_i = 0, \cdots, 10}$

- In the inner mesh points, $\mathbf{x_i = 1, \cdots, 9}$ the discretization of the differential equation $\mathbf{y''(x) = 2y}$ provides the following set of equations:

$$2y_i = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} \qquad (i = 1, \cdots, 9)$$

$$\boxed{y_{i+1} - 2y_i(1+h^2) + y_{i-1} = 0} \qquad (i = 1, \cdots, 9)$$

  till now we have $\mathbf{9}$ equations for $\mathbf{11}$ $(\mathbf{y_i = y_0, \cdots, y_{10}})$ unknowns

- an additional equation is provided by the first boundary condition

$$\boxed{y(0) = 1} \qquad (i = 0)$$

- other equation is provided by the other boundary condition

$$\boxed{y'(1) = 0} \qquad \frac{y_{11} - y_9}{2h} = 0 \quad \Rightarrow \quad y_{11} = y_9$$

  and the discretized differential equation defined on the last mesh point $\mathbf{i = 10}$

$$y_{11} - 2y_{10}(1+h^2) + y_9 = 0 \qquad (\text{as, } y_{11} = y_9)$$
$$y_9 - 2y_{10}(1+h^2) + y_9 = 0$$

$$\boxed{y_9 - y_{10}(1+h^2) = 0}$$

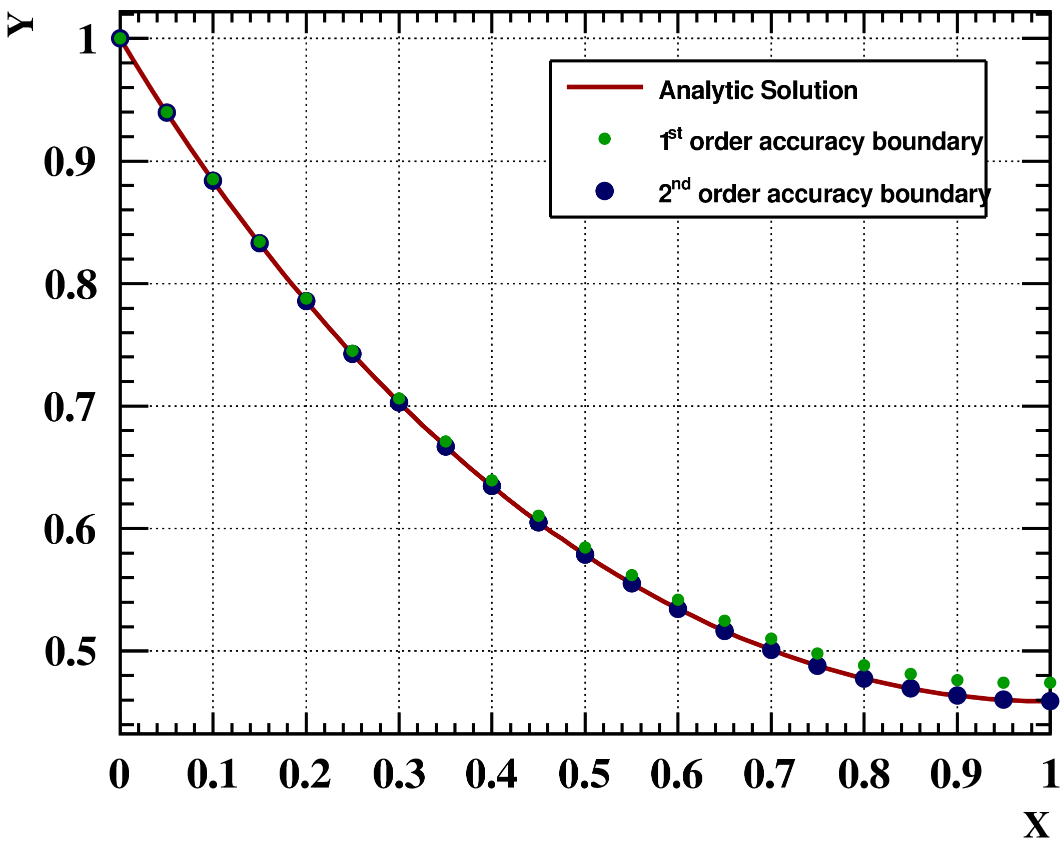
finite-difference method: example

the system of equations to solve (using for instance LU decomposition)

$$
\begin{aligned}
i = 1 \quad &: \quad -2(1+h^2)y_1 + y_2 &= -y_0 \\
i = 2 \quad &: \quad y_1 - 2(1+h^2)y_2 + y_3 &= 0 \\
i = 3 \quad &: \quad y_2 - 2(1+h^2)y_3 + y_4 &= 0 \\
&\quad \vdots &= \vdots \\
i = 9 \quad &: \quad y_8 - 2(1+h^2)y_9 + y_{10} &= 0 \\
\text{boundary condition eq} \quad &: \quad y_9 - (1+h^2)y_{10} &= 0
\end{aligned}
$$

$$
\begin{pmatrix}
-2(1+h^2) & +1 & 0 & 0 & 0 & \cdots & 0 & 0 \\
+1 & -2(1+h^2) & +1 & 0 & 0 & \cdots & 0 & 0 \\
0 & +1 & -2(1+h^2) & +1 & 0 & \cdots & 0 & 0 \\
\vdots & & \vdots & & & & & \vdots \\
0 & 0 & 0 & 0 & 0 & \cdots & +1 & (1+h^2)
\end{pmatrix}
\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{10} \end{pmatrix}
=
\begin{pmatrix} -y_0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}
$$

finite-differ method: example (cont.)



Heat conduction in rod

- ✔ We are going to solve the stationary heat equation for a cylindrical rod of length L:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) T = 0$$

- ✔ it is a one-dimensional problem if the rod cylinder is perfectly isolated

$$\frac{d^2T}{dx^2} = 0 \quad x \in [0, L]$$
$$T(x=0) = T_a$$
$$T(x=L) = T_b$$

- ✔ Analytical solution:

$$T(x) = T_a + \frac{T_b - T_a}{L} x$$

Numerical solution

Let's use 6 grid points: $n = 0, ..., 5$

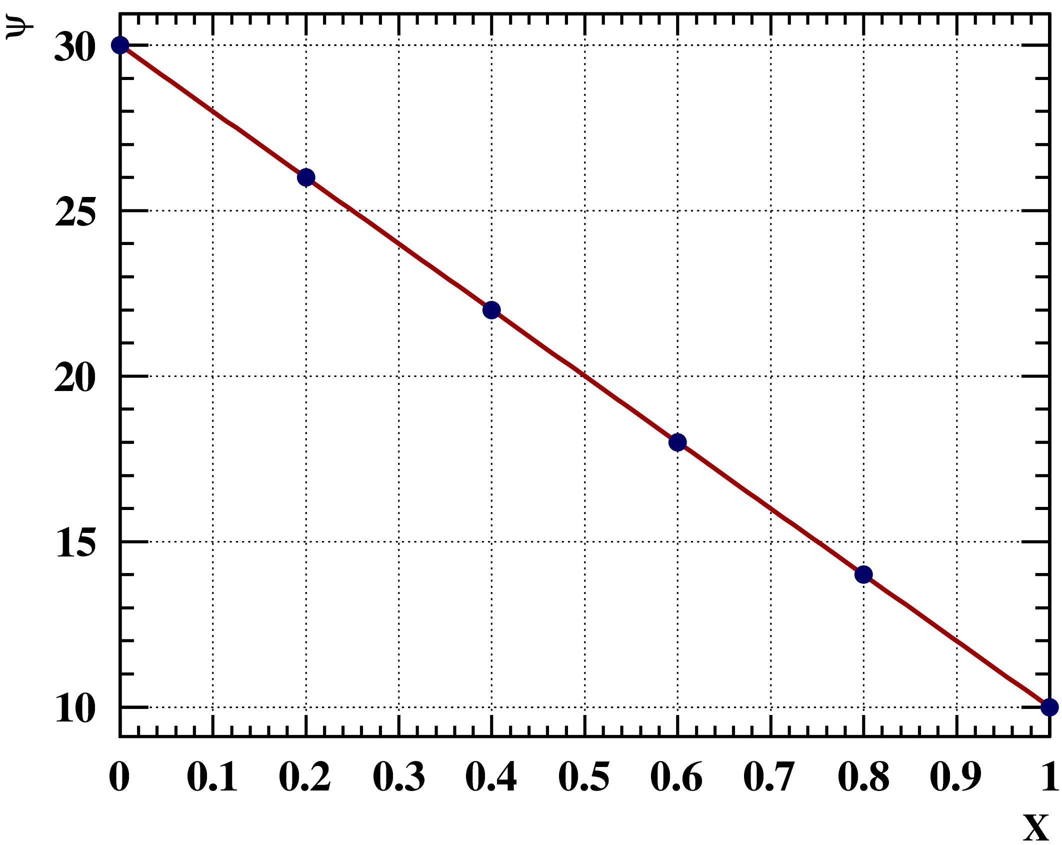
$T_{n+1} - 2T_n + T_{n-1} = 0$ (n=1,...,4)

boundary values: $T_0 = T_a$ and $T_5 = T_b$

$$\begin{aligned} T_2 - 2T_1 + T_0 &= 0 \quad \text{(n=1)} \\ T_3 - 2T_2 + T_1 &= 0 \quad \text{(n=2)} \\ T_4 - 2T_3 + T_2 &= 0 \quad \text{(n=3)} \\ T_5 - 2T_4 + T_3 &= 0 \quad \text{(n=4)} \end{aligned}$$

$$\begin{bmatrix} -2 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & +1 \\ 0 & 0 & +1 & -2 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \end{bmatrix} = \begin{bmatrix} -T_a \\ 0 \\ 0 \\ -T_b \end{bmatrix}$$

Heat equation: finite-differences



other examples

✔ schrodinger equation

$$-\frac{h^2}{4\pi^2 m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$

✔ Poisson equation

$$\frac{d^2\phi}{dx^2} = f(x)$$

Computational Physics

Partial Differential

Equations

Fernando Barao, Phys Department IST (Lisbon)

Partial Differential Equations

- Physical quantities vary in time and space

  $u(t, x, y)$

- The most general form for a two-independent variable partial derivative equation

$$a\frac{\partial^2 u}{\partial x^2} + 2b\frac{\partial^2 u}{\partial x \partial y} + c\frac{\partial^2 u}{\partial y^2} + f(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}) = 0$$

- one distinguish three types of equations

hyperbolic	$ac - b^2 < 0$
parabolic	$ac - b^2 = 0$
elliptic	$ac - b^2 > 0$

hyperbolic	
$c^2 \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial t^2} = f(t, x)$	wave eq
$c^2 \frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial t^2} - a\frac{\partial u}{\partial t} = f(t, x)$	wave damping
parabolic	
$D\frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial t} = f(t, x)$	diffusion eq
elliptic	
$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\rho(t, x)$	Poisson eq
$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - \frac{2m}{\hbar^2} U(x) = 0$	Schroedinger eq

Poisson equation

- Maxwell equations relate electromagnetic fields ($\vec{E}$ and $\vec{B}$) with theirs sources (charges and electric currents)

- The **Poisson equation** relates the electric potential **($\varphi(\vec{r})$)** with the electric charge distribution **($\rho(\vec{r})$)**

$$\begin{cases} \nabla \cdot \vec{E}(\vec{r}) & = \frac{\rho(\vec{r})}{\varepsilon_0} \\ \vec{E}(\vec{r}) & = -\nabla\varphi(\vec{r}) \end{cases}$$

$$\boxed{\nabla^2\varphi = \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2} = -\frac{\rho(\vec{r})}{\varepsilon_0}}$$

- The **laplace equation**:

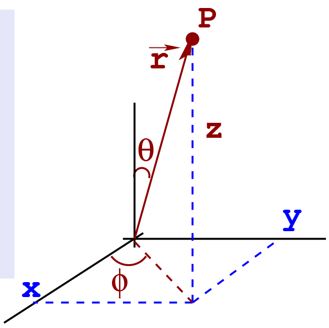
$$\boxed{\nabla^2\varphi = \frac{\partial^2\varphi}{\partial x^2} + \frac{\partial^2\varphi}{\partial y^2} + \frac{\partial^2\varphi}{\partial z^2} = 0}$$

spherical coordinates

r = radius

θ = polar angle

ϕ = azimuthal angle



Laplace equation:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial V}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial V}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 V}{\partial\phi^2} = 0$$

Potencial only function of r:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial V}{\partial r}\right) = 0 \quad\Rightarrow\quad r^2\frac{\partial V}{\partial r} = k \quad\Rightarrow\quad \frac{\partial V}{\partial r} = \frac{k}{r^2}$$

$$V(r) = -\frac{k}{r} + b \qquad [V(r = \infty) = 0 \Rightarrow b = 0]$$

$$\boxed{V(r) = -\frac{k}{r}}$$

Poisson equation: numerical solution

ONE-DIMENSIONAL PROBLEM

$$\frac{d^2V}{dx^2} = f(x)$$

$$\frac{V(x_n-h)-2V(x_n)+V(x_n+h)}{h^2} = f(x_n)$$

$$V_{n-1} - 2V_n + V_{n+1} = h^2 f_n$$

inner grid points: $n = 1, 2, \cdots, N-1$

Boundary conditions:

$V(x = x_0) = V_0$

$V(x = x_N) = V_1$

Set of equations

$(n = 1)$ $\quad V_0 - 2V_1 + V_2 = h^2 f_1$

$(n = 2)$ $\quad V_1 - 2V_2 + V_3 = h^2 f_2$

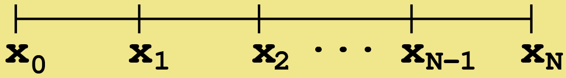
$\vdots \quad \vdots$

$(n = N-1)$ $\quad V_{N-2} - 2V_{N-1} + V_N = h^2 f_{N-1}$

discretization

N intervals: $N+1$ grid points

$n = 0, 1, 2, \cdots, N$



matrix equations

unknows: $V_1, V_2, \cdots, V_{N-1}$

$$\begin{pmatrix} -2 & +1 & 0 & 0 & \cdots & \\ +1 & -2 & +1 & 0 & \cdots & \\ 0 & +1 & -2 & +1 & \cdots & \\ & \ddots & \ddots & \ddots & & \\ & & & & +1 & -2 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ \vdots \\ V_{N-1} \end{pmatrix} = \begin{pmatrix} h^2 f_1 - V_0 \\ h^2 f_2 \\ h^2 f_3 \\ \vdots \\ h^2 f_{N-1} - V_N \end{pmatrix}$$

Poisson equation: numerical solution

TWO-DIMENSIONAL PROBLEM

$$\frac{\partial^2\varphi(x,y)}{\partial x^2} + \frac{\partial^2\varphi(x,y)}{\partial y^2} = -\frac{\rho(x,y)}{\varepsilon_0} = f(x,y)$$

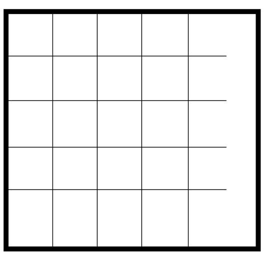
$$\frac{\partial^2\varphi}{\partial x^2} = \frac{V(x-h,y)-2V(x,y)+V(x+h,y)}{h^2} = \frac{V(i-i,j)-2V(i,j)+V(i+1,j)}{h^2}$$

$$\frac{\partial^2\varphi}{\partial y^2} = \frac{V(x,y-h)-2V(x,y)+V(x,y+h)}{h^2} = \frac{V(i,j-1)-2V(i,j)+V(i,j+1)}{h^2}$$

$$V(i,j-1) + V(i,j+1) + V(i-1,j) + V(i+1,j) - 4V(i,j) = h^2\ f(i,j)$$

$i = 1, 2, \cdots, N-1$

$j = 1, 2, \cdots, M-1$



grid boundaries

Boundary conditions:

$V(i = 0, j) = V_{0_i}$ $\quad V(i, j = 0) = V_{1_i}$

$V(i = N, j) = V_{0_e}$ $\quad V(i, j = M) = V_{1_e}$

discretization

N^2 intervals:

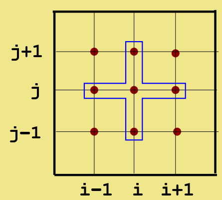
$(N+1) \times (N+1)$ points

x coordinate:

$i = 0, 1, 2, \cdots, N$

y coordinate:

$j = 0, 1, 2, \cdots, M$



Poisson equation (2-dim)

✔ A set of $(N-1)^2$ equations in $(N-1)^2$ unknowns can be established, involving the boundary values:

$\boxed{j=1}$

$i=1$	$V(1,0)+V(1,2)+V(0,1)+V(2,1)-4V(1,1)=h^2f(1,1)$
$i=2$	$V(2,0)+V(2,2)+V(1,1)+V(3,1)-4V(2,1)=h^2f(2,1)$
$i=3$	$V(3,0)+V(3,2)+V(2,1)+V(4,1)-4V(3,1)=h^2f(3,1)$
$\vdots$	$\vdots$
$i=N-1$	$V(N-1,0)+V(N-1,2)+V(N-2,1)+V(N,1)-4V(N-1,1)=h^2f(N-1,1)$
$\vdots$	$\vdots$

$\boxed{j=N-1}$

$i=1$	$V(1,N-2)+V(1,N)+V(0,N-1)+V(2,N-1)-4V(1,N-1)=h^2f(1,N-1)$
$i=2$	$V(2,N-2)+V(2,N)+V(1,N-1)+V(3,N-1)-4V(2,N-1)=h^2f(2,N-1)$
$\vdots$	$\vdots$

Our unknowns:

$\boxed{V(1,1)\ V(2,1)\ V(2,1)\cdots V(N-1,1)\ V(1,2)\ V(2,2)\ V(3,2)\cdots V(N-1,2)\ V(1,3)\ V(2,3)\cdots}$

Poisson equation (2-dim)

the linear system to solve

$\boldsymbol{A\cdot v=b}$

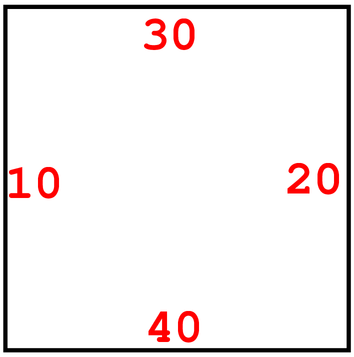
involves a pentadiagonal matrix A:

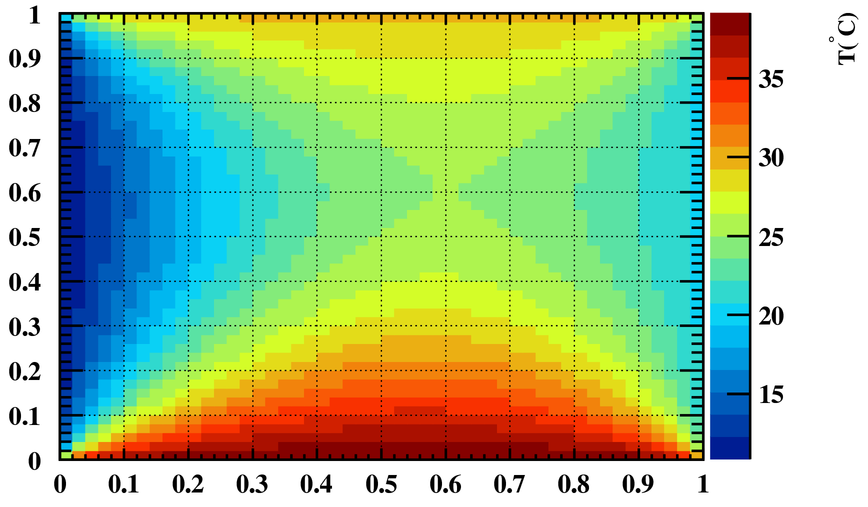
$$\begin{pmatrix} -4 & +1 & 0 & \cdots & 0 & +1 & 0 & \cdots \\ +1 & -4 & +1 & & & & +1 & \\ 0 & +1 & -4 & +1 & & & & +1 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 1 & & & & & & & \\ & \ddots & & & & & & \\ \vdots & & & & & & & \end{pmatrix} \begin{pmatrix} V(1,1) \\ V(2,1) \\ V(3,1) \\ \vdots \\ V(N-1,1) \\ V(1,2) \\ \vdots \end{pmatrix} = \begin{pmatrix} h^2f(1,1)-V(1,0)-V(0,1) \\ h^2f(2,1)-V(2,0) \\ h^2f(3,1)-V(3,0) \\ \vdots \\ \\ \\ \end{pmatrix}$$

Heat equation: example

Suppose we have a metallic plate with every side at different temeperature

Temperature required to be 10, 20, 30, 40 degrees on boundaries





distribution of temperatures in the plate

Poisson eq: example

Suppose we have a metallic plate grounded ($V = 0$) and in its center an electric charge

Electric potential required to be zero on boundaries