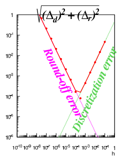
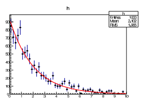
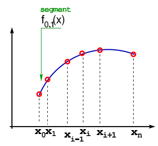
Computational Physics

numerical methods with C++ (and UNIX)







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Computational Physics

Physics problems

and Solutions

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Numerical methods

- ✔ Solving Ordinary Differential Equations
  - Euler method
  - Runge-Kutta method
  - examples

ODEs: boundary value problems

✔ There are problems in physics where differential equations conditions are given at the boundaries.

Suppose for instance a rod that is conducting heat from two reservoirs at different temperatures, $T(x=0) = T_0$ and $T(x=L) = T_L$

The temperature equation in the bar:

$$\frac{\partial T}{\partial t} = \frac{k}{c\rho}\frac{\partial^2 T}{\partial x^2}$$

k, thermal conductivity (W.m^{-1}.K^{-1})
c, specific heat capacity (J.Kg^{-1})
ρ, density (Kg.m^{-3})

✔ In equilibrium ($\frac{\partial T}{\partial t} = 0$), the temperature equation is an example of a linear 2nd-order boundary value problem:

$$a_2(x)\, y''(x) + a_1(x)\, y'(x) + a_0(x)\, y(x) = f(x)\ , \qquad x \in [a,b]$$
$$\alpha_0 y(a) + \alpha_1 y'(a) = \lambda_1\ , \qquad |\alpha_0| + |\alpha_1| \neq 0$$
$$\beta_0 y(b) + \beta_1 y'(b) = \lambda_2\ , \qquad |\beta_0| + |\beta_1| \neq 0$$

BV problems: finite-differences

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

  grid spacing $h = \frac{b-a}{N-1}$

- ✔ using the central difference derivative for the grid points $k = 2, \cdots, N-1$

$$\begin{aligned} y''(x_k) \equiv y''_k &\simeq \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} \\ y'(x_k) \equiv y'_k &\simeq \frac{y_{k+1} - y_{k-1}}{2h} \end{aligned}$$

- ✔ the differential equation becomes for inner grid points, $k = 2, \cdots, N-1$

$$\begin{aligned} a_2(x)\, y''(x) + a_1(x)\, y'(x) + a_0(x)\, y(x) &= f(x) \\ a_k \frac{y_{k+1} - 2y_k + y_{k-1}}{h^2} + b_k \frac{y_{k+1} - y_{k-1}}{2h} + c_k y_k &= f_k \end{aligned}$$

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

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

BV problems: finite-differences (cont.)

- ✔ the boundary problem reduces to a system of inhomogeneous linear equations:

$$\begin{cases} \left(\frac{a_2}{h^2} - \frac{b_2}{2h}\right) y_1 + \left(c_2 - 2\frac{a_2}{h^2}\right) y_2 + \left(\frac{a_2}{h^2} + \frac{b_2}{2h}\right) y_3 = f_2 & \text{(k=2)} \\ \left(\frac{a_3}{h^2} - \frac{b_3}{2h}\right) y_2 + \left(c_3 - 2\frac{a_3}{h^2}\right) y_3 + \left(\frac{a_3}{h^2} + \frac{b_3}{2h}\right) y_4 = f_3 & \text{(k=3)} \\ \cdots = \cdots & \\ \left(\frac{a_{N-1}}{h^2} - \frac{b_{N-1}}{2h}\right) y_{N-2} + \left(c_3 - 2\frac{a_{N-1}}{h^2}\right) y_{N-1} + \left(\frac{a_{N-1}}{h^2} + \frac{b_{N-1}}{2h}\right) y_N = f_{N-1} & \text{(k=N-1)} \end{cases}$$

$$\begin{cases} \left(c_2 - 2\frac{a_2}{h^2}\right) y_2 + \left(\frac{a_2}{h^2} + \frac{b_2}{2h}\right) y_3 = f_2 - \left(\frac{a_2}{h^2} - \frac{b_2}{2h}\right) y_1 \\ \left(\frac{a_3}{h^2} - \frac{b_3}{2h}\right) y_2 + \left(c_3 - 2\frac{a_3}{h^2}\right) y_3 + \left(\frac{a_3}{h^2} + \frac{b_3}{2h}\right) y_4 = f_3 \\ \cdots = \cdots \\ \left(\frac{a_{N-1}}{h^2} - \frac{b_{N-1}}{2h}\right) y_{N-2} + \left(c_3 - 2\frac{a_{N-1}}{h^2}\right) y_{N-1} = f_{N-1} - \left(\frac{a_{N-1}}{h^2} + \frac{b_{N-1}}{2h}\right) y_N \end{cases}$$

- ✔ in matrix notation

$$\begin{bmatrix} B_2 & C_2 & 0 & \cdots & 0 \\ A_3 & B_3 & C_3 & 0 & \cdots \\ 0 & A_4 & B_4 & C_4 & \cdots \end{bmatrix} \begin{bmatrix} y_2 \\ y_3 \\ \cdots \end{bmatrix} = \begin{bmatrix} f_2 - \left(\frac{a_2}{h^2} - \frac{b_2}{2h}\right) y_1 \\ f_3 \\ \cdots \end{bmatrix}$$

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

$$\frac{d^2T}{dx^2} = 0 \quad x \in [0, L]$$
$$T(x=0) = T_0$$
$$T(x=L) = T_L$$

- Analytical solution:

$$T(x) = T_0 + \frac{T_L - T_0}{L} x$$

Numerical solution

Let's use 6 grid points: $n = 1, ..., 6$

$T_{n+1} - 2T_n + T_{n-1} = 0$ (n=2,5)

boundary values: $T_1 = T_0$ and $T_6 = T_L$

$$\begin{aligned} T_3 - 2T_2 + T_1 &= 0 \quad \text{(n=2)} \\ T_4 - 2T_3 + T_2 &= 0 \quad \text{(n=3)} \\ T_5 - 2T_4 + T_3 &= 0 \quad \text{(n=4)} \\ T_6 - 2T_5 + T_4 &= 0 \quad \text{(n=5)} \end{aligned}$$

$$\begin{bmatrix} -2 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & +1 \\ 0 & 0 & +1 & -2 \end{bmatrix} \begin{bmatrix} T_2 \\ T_3 \\ T_4 \\ T_5 \end{bmatrix} = \begin{bmatrix} -T_0 \\ 0 \\ 0 \\ -T_L \end{bmatrix}$$

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

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