Advanced Methods on Computational Physics

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Exercise Set 9

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Run the programs by using 'main9.sh' script file; 'armadillo' and 'openblas' libraries are required.

1.

If the rod has insulated endpoints the boundary conditions become

$$\frac{\partial T}{\partial x}(t, x = 0) = \frac{\partial T}{\partial x}(t, x = 10) = 0\,, T(t = 0, x) = e^{-x/5}$$

Therefore

$$\frac{\partial T}{\partial t}(t, x) = K\frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}(t, x)\right) = \frac{K}{\Delta x}\left[\frac{\partial T}{\partial x}(t, x + \Delta x) - \frac{\partial T}{\partial x}(t, x)\right]$$

And

$$\frac{\partial T}{\partial x}(t + \Delta t, x) = \frac{T(t + \Delta\mathrm{t}, \mathrm{x} + \Delta\mathrm{x}) - T(t + \Delta t, x)}{\Delta x}$$

By calculating $T(t, x)$ we see that as time pass, T goes to ∞ or $-\infty$ because there is no temperature flux at endpoints.

2.

$$< v_z^2 >= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(\frac{\beta m}{2\pi}\right)^{\frac{3}{2}} v_z^2 \exp(-\frac{\beta m\left(v_x^2 + v_y^2 + v_z^2\right)}{2})\mathrm{d}v_x\mathrm{d}v_y\mathrm{d}v_z$$

Assume $A = \left(\frac{\beta m}{2\pi}\right)^{3/2}, \alpha = \frac{\beta m}{2}$ and by using spherical coordinates we have

$$v_x = r\cos\phi\sin\theta\,, v_y = r\sin\phi\sin\theta\ \,, v_z = r\cos\theta\,, dv_x dv_y dv_z = r^2\sin\theta dr d\phi d\theta$$

$$< v_z^2 > = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi\, A\, r^4\sin\theta\cos^2\theta\exp -\alpha r^2$$

$$< v_z^2 > = 2\pi A\int_0^{\pi}\sin\theta\cos^2\theta\,\mathrm{d}\theta\int_0^{\infty} r^4 e^{-\alpha r^2}\mathrm{d}r$$

$$u = \cos\theta \to \mathrm{d}u = -\sin\theta\,\mathrm{d}\theta \Rightarrow \int_0^{\pi} \sin\theta \cos^2\theta\,\mathrm{d}\theta \;= -\int u^2 \mathrm{d}u = -\frac{u^3}{3} = (\cos^3 0 - \cos^3\pi)/3 = \frac{2}{3}$$

$$< v_z^2 >= \frac{4}{3}\pi A \int_0^{\infty} r^4 e^{-\alpha r^2}\,\mathrm{d}r$$

Now we can calculate this integral with Monte Carlo method. In theory the answer should be

$$I = \int_0^{\infty} e^{-\alpha r^2} \mathrm{d}r = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}} \Rightarrow$$

$$< v_z^2 >= \frac{4}{3}\pi A \frac{\partial^2 I}{\partial \alpha^2} = \frac{1}{2}\pi^{\frac{3}{2}} A \alpha^{-\frac{5}{2}}$$

3.

$$y''(t) + a y'(t) + \omega^2 y(t) = \cos\omega t$$

$$y(0) = A, y'(0) = 0$$

Analytically we have

Homogeneous equation

$$y''(t) + a y'(t) + \omega^2 y(t) = 0$$

$$\to \lambda^2 + a\lambda + \omega^2 = 0 \to \lambda = -\frac{a}{2} \pm \sqrt{a^2 - 4\omega^2}$$

$$y_h(t) = \begin{Bmatrix} A_1 e^{-\frac{a}{2}t} + B_1 t e^{-\frac{a}{2}t} \;,\; a = 2\omega \\ (A_2 e^{\sqrt{a^2-4\omega^2}t} + B_2 e^{-\sqrt{a^2-4\omega^2}t}) e^{-\frac{a}{2}t} \;, \quad |a| > 2\omega \\ (A_3 \cos\sqrt{4\omega^2 - a^2}t + B_3 \sin(\sqrt{4\omega^2 - a^2})t) e^{-\frac{a}{2}t} \;, \; |a| < 2\omega \end{Bmatrix}$$

$$y_p = \frac{1}{\mathrm{a}\omega} \sin\omega t$$

$$y = y_h + y_p$$

Suppose $a = 2\omega$

$$y(t) = A_1 e^{\lambda t} + B_1 t e^{\lambda t} + \frac{1}{a\omega}\sin\omega t$$
$$y(0) = A \to A_1 = A$$
$$y'(t) = A\lambda e^{\lambda t} + B_1 e^{\lambda t} + B_1 \lambda t e^{\lambda t} + \frac{1}{a}\cos\omega t$$
$$y'(0) = 0 \to A + B_1 + \frac{1}{a} = 0 \to B1 = -A - \frac{1}{a}$$
$$\Rightarrow y(t) = \left((1-t)A + \frac{t}{a}\right) e^{-\frac{a}{2}t} + \frac{1}{a\omega}\sin\omega t$$

For solving this equation numerically suppose $p(t)$ as

$$p(t) = y'(t) \rightarrow \frac{\mathrm{d}p(t)}{\mathrm{d}t} = y''(t) = \cos\omega t - ap(t) - \omega^2 y(t) = f(t, y(t), p(t))$$

- Euler Method

$$y(t + \Delta t) = y(t) + p(t)\Delta t$$

$$p(t + \Delta t) = p(t) + f(t, y(t), p(t))\Delta t = p(t) + (\cos\omega t - ap(t) - \omega^2 y(t))\Delta t$$

$$\rightarrow p(t + \Delta t) = (1 - a\Delta t)p(t) + \Delta t \cos\omega t - \omega^2 \Delta t\, y(t)$$

- RF4 Method

$$y(t + \Delta t) = y(t) + \frac{\Delta t}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$p(t + \Delta t) = p(t) + \frac{\Delta t}{6}(m_1 + 2m_2 + 2m_3 + m_4)$$

And

$$k_1 = p(t), m_1 = f(t, y(t), p(t)) = (\cos\omega t - ap(t) - \omega^2 y(t)$$

$$k_2 = p(t) + \frac{m_1}{2}\ , m_2 = f\left(t + \frac{\Delta t}{2}, y(t) + \frac{k_1}{2}, p(t) + \frac{m_1}{2}\right)$$

$$k_3 = p(t) + \frac{m_2}{2}\ , m_3 = f\left(t + \frac{\Delta t}{2}, y(t) + \frac{k_2}{2}, p(t) + \frac{m_2}{2}\right)$$

$$k_4 = p(t) + m_3\ , m_4 = f(t + \Delta t, y(t) + k_3, p(t) + m_3)$$

4.

- Finite Difference Method

$$y''(t) = p(t)y'(t) + g(t)y(t) + r(t)$$

$$y(t_{fin}) = \beta, y(t_{init}) = \alpha, \Delta t = \frac{t_{fin} - t_{init}}{N}$$

We can calculate $y(t)$ by solving this system of equations

$$D^{(N-1\times N-1)}W^{(N-1\ \times 1)} = C^{(N-1\ \times 1)}$$

Where W, C and D are

$$W_i = y(t_{init} + i\Delta t)$$

$$C_i = -\Delta t^2 r(t_{init} + i\Delta t) + \left[e_0\delta_{i1} + e_N\delta_{i,N-1}\right]\ , e_0 = \left[-\frac{\Delta t}{2}p(t_{init} + \Delta t) + 1\right]\alpha,$$

$$, e_N = \left[-\frac{\Delta t}{2}p\left(t_{finit} - \Delta t\right) + 1\right]\beta$$

$$D_{ij} = \left\{[2 + \Delta t^2 g(t_{init} + i\Delta t)]\delta_{i,j} + \left[\frac{\Delta t}{2} p(t + i\Delta t) - 1\right] \delta_{i,j-1} + \left[-\frac{\Delta t}{2} p(t + i\Delta t) - 1\right] \delta_{i,j+1}\right\}$$

Now we can solve our equation by placing

$$t_{init} = 0, t_{fin} = 10, N = 1000$$

$$p(t) = -a, g(t) = -\omega^2, r(t) = \cos \omega t$$

$$\alpha = A, \beta = y_{theory}(t_{fin})$$