PHYS4070

Week 11 Worksheet — The One-Dimensional Heat Equation (Part II)

OBJECTIVES

- write an RK4 algorithm that solves a partial differential equation which is first-order in time
- appreciate the relationship between RK4 stability, time step, and grid resolution

BACKGROUND

In this workshop, we will employ the fourth-order Runge–Kutta (RK4) method to solve for the dynamics of the heat conduction in a copper rod of length L, with a Gaussian initial condition (refer to Part I of the worksheet for additional details):

$$\frac{\partial u(x,t)}{\partial t} = \alpha \frac{\partial^2 u(x,t)}{\partial x^2}\,, \qquad u(x,0) = \frac{U_0}{a\sqrt{\pi}} \exp\left(-\frac{x^2}{a^2}\right). \tag{1}$$

The ends of the rod are held constant at $u(-L/2,t) = u(L/2,t) = 0$ throughout the dynamics.

Previously, we showed that Eq. (1) can be rewritten in dimensionless form:

$$\frac{\partial \bar{u}(\bar{x},\bar{t})}{\partial \bar{t}} = \frac{\partial^2 \bar{u}(\bar{x},\bar{t})}{\partial \bar{x}^2}\,, \qquad \bar{u}(\bar{x},0) = \frac{1}{\sqrt{\pi}} \exp\left(-\bar{x}^2\right), \tag{2}$$

where $\bar{x} = x/a$, $\bar{t} = \alpha t/a^2$, and $\bar{u} = au/U_0$.

We also implemented a second-order central difference method to approximate the second derivative in Eq. (2):

$$f''(\bar{x}) \approx \frac{f(\bar{x}+\Delta\bar{x}) - 2f(\bar{x}) + f(\bar{x}-\Delta\bar{x})}{(\Delta\bar{x})^2}\,. \tag{3}$$

Next, we will solve Eq. (2) by dividing the "$(\bar{x},\bar{t})$" space into a regular grid, and then propagating the vector $\bar{\mathbf{u}}(\bar{t}) = [\bar{u}(-\bar{L}/2,\,\bar{t}),\ \bar{u}(-\bar{L}/2+\Delta\bar{x},\,\bar{t}),\ \bar{u}(-\bar{L}/2+2\Delta\bar{x},\,\bar{t}),\ \ldots,\ \bar{u}(\bar{L}/2,\,\bar{t})]$ through time in discrete time steps using an RK4 algorithm. Here, $\bar{L} = L/a$ is the dimensionless size of the system.

QUESTIONS

(a) Combine your second-order central difference spatial derivative from the previous workshop with the formula for an RK4 algorithm (see the lecture from Week 6) to numerically solve for the dynamics of the vector $\bar{\mathbf{u}}(\bar{t})$ with $\bar{L} = 20$.

(b) The analytical solution to Eq. (2) for $\bar{L} \to \infty$ can be obtained by using the Green's function method, and is given by

$$\bar{u}_{\text{anal}}(\bar{x},\bar{t}) = \frac{1}{\sqrt{\pi}} \frac{\exp[-\bar{x}^2/(1+4\bar{t})]}{\text{sqrt}(1+4\bar{t})}\,. \tag{4}$$

Plot the normalised root-mean-square error between your numerical solution $\bar{u}_{\text{num}}$ and Eq. (4),

$$\text{err}(\bar{t}) = \sqrt{\frac{\sum_n [\bar{u}_{\text{num}}(\bar{x}_n,\bar{t}) - \bar{u}_{\text{anal}}(\bar{x}_n,\bar{t})]^2}{\sum_n \bar{u}_{\text{anal}}(\bar{x}_n,\bar{t})^2}}\,, \tag{5}$$

as a function of $\bar{t}$, where $\bar{x}_n$ are your grid points.

How does the accuracy at a given time $\bar{t}$ scale with your time step $\Delta\bar{t}$? Why? At what time step $\Delta\bar{t}_{\max}$ does your numerical solution "blow up"? Repeat this for multiple grid resolutions $\Delta\bar{x}$, and plot $\Delta\bar{t}_{\max}$ versus $\Delta\bar{x}$. What do you observe? The spatial derivative in Eq. (2) can be "diagonalized" by using a Fourier transform, $\mathcal{F}$: $\partial^2/\partial\bar{x}^2 \longrightarrow -\bar{k}^2$. Thus, the elements of $\mathcal{F}\bar{\mathbf{u}} = \bar{\mathbf{u}}_{\mathcal{F}}$ decouple. The element of $\bar{\mathbf{u}}_{\mathcal{F}}$ with the maximum magnitude of $\bar{k}$ evolves the most rapidly: $\partial\bar{u}_{\mathcal{F}}(\bar{k}_{\max}, \bar{t})/\partial\bar{t} = -\bar{k}_{\max}^2\bar{u}_{\mathcal{F}}(\bar{k}_{\max}, \bar{t})$, where $\bar{k}_{\max} = \pi/\Delta\bar{x}$. Hence, explain why $\Delta\bar{t}_{\max}$ varies with $\Delta\bar{x}$.

USEFUL TIPS

Use "#include <cmath>" to utilize mathematical functions. You can define π at the beginning of your code as "const double pi = 4 * atan(1)".