Homework #3

ME 5311 – Spring 2023

8 February 2023

1 Constructing finite difference approximations [4 points]

For a grid with constant Δx spacing as in Figure 1, we will construct a finite difference approximation of the first derivative at location i using values $u_{i-1/2}$, $u_{i+1/2}$, and $u_{i+3/2}$.

Derive a finite-difference approximation to the first derivative at i of the form:

$$\frac{\partial u}{\partial x}|_i = \frac{1}{\Delta x}(a\,u_{i-1/2} + b\,u_{i+1/2} + c\,u_{i+3/2}). \tag{1}$$

We will use two ways to find the constants a, b, and c.

a. Find a, b, and c, the leading error term, and the order of accuracy using a Taylor table.

b. Find a, b, and c by first constructing a Lagrange interpolating polynomial and then differentiating polynomial at x_i. Does the solution agree with the result of part a? Is the order of the polynomial consistent with the order of accuracy of the method?

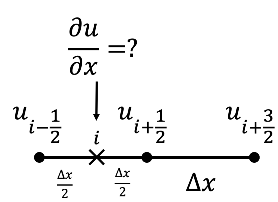

Figure 1: Variable placement on the computational grid for the first derivative approximation.

2 Simpson's Rule Again! [2 points]

We will use our Simpson's rule implementation from last week to integrate another function. The error estimate for Simpson's rule is

$$E = -\frac{1}{90}\Delta x^5 f^{(4)}(\xi), \tag{2}$$

where $f^{(4)}$ is the fourth derivative of the integrand function and ξ is somewhere between the two integration bounds.

This week we will integrate $\int_0^1 \sqrt{x}\,\mathrm{d}x$.

a. Numerically integrate $\int_0^1 \sqrt{x}\,\mathrm{d}x$ and estimate the convergence rate.

b. Explain the result you found in (a).

3 Runge–Kutta Method [4 points]

We will use the low-storage third-order Runge–Kutta scheme of Spalart, Moser & Rogers (1991) we discussed in class to numerically integrate a couple of ODEs. To advance the solution u from time t to $t + \Delta t$, three sub-steps, are taken. If the solution at time t is u_n the following three steps are taken to advance the solution to u_{n+1} at $t + \Delta t$:

$$u_{n+\alpha} = u_n + \Delta t \, \frac{8}{15} \, f(u_n) \tag{3}$$

$$u_{n+\alpha_1} = u_{n+\alpha} + \Delta t \left(-\frac{17}{60} f(u_n) + \frac{5}{12} f(u_{n+\alpha}) \right) \tag{4}$$

$$u_{n+1} = u_{n+\alpha_1} + \Delta t \left(-\frac{5}{12} f(u_{n+\alpha}) + \frac{3}{4} f(u_{n+\alpha_1}) \right) \tag{5}$$

a. Numerically integrate

$$\frac{\mathrm{d}u}{\mathrm{d}t} = u. \tag{6}$$

with $u(0) = 1$ the initial condition up to $t_{\text{end}} = 2$ and show that the convergence rate is third-order. Use the 2-norm to calculate the error.

b. Repeat the convergence rate of (a) but using the 1-norm this time. Show that the error values are different, but the convergence rate does not change.

c. Numerically integrate the Lorenz system:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \sigma(y - x), \tag{7}$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = x(\rho - z) - y, \tag{8}$$

$$\frac{\mathrm{d}z}{\mathrm{d}t} = xy - \beta z, \tag{9}$$

where β, ρ, and σ are scalar constants. We will use $\beta = 8/3$, $\rho = 26$, and $\sigma = 11$ because for these values the system exhibits chaotic behavior. Use an initial condition ($t = 0$) close to $x = y = z = 1$ and integrate to $t = 40$. Plot the trajectory of $(x,\ y,\ z)$. In part a, u was a scalar, but here u is the vector $\mathbf{u} = [x, y, z]$. Thus, both u and $f(u)$ are vectors and we can write (7–9) as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = f(\mathbf{u}). \tag{10}$$

where

$$\mathbf{u} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{11}$$

and

$$f(\mathbf{u}) = \begin{bmatrix} \sigma(y - x) \\ x(\rho - z) - y \\ xy - \beta z \end{bmatrix} \tag{12}$$

d. Perform a second integration by slightly changing the initial condition, say $x_{new} = 1.001 x_{old}$. Plot the difference as a function of time between the two integrations, i.e., the distance between $(x_1,\ y_1,\ z_1)$ and $(x_2,\ y_2,\ z_2)$.