CO906 worksheet 1

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1 Individual work

1.1 Getting started with the CSC computing environment

This task is just to make sure that everyone can run the example codes and plot the results.

- Download and unpack the tarball worksheet1-Q1.1.tgz from the class website.
- Compile the code and link to the gsl library using the Makefile provided.
- Run the code on the CoW by appropriately modifying the PBS script provided.
- The code produces a file containing plots of the functions $\mathrm{erf}(t)$, $t\,\mathrm{erf}(t)$ and $t^2\,\mathrm{erf}(t)$.

The sample code, while performing a trivial task, illustrates a large number of concepts and techniques which will be useful generally:

- Linking functions (in this case, erf) from an external library (in this case, GSL).
- How to split a large code into several files.
- Using make to automate complicated compilation and linking tasks.
- How to submit jobs to the CoW using PBS.
- Reading command line arguments into a code
- Dynamic memory allocation using calloc();
- How to read parameters from an external file.
- How to get a program to time itself.
- Producing output at fixed time intervals even as the time increment varies.

Questions

(a) Plot the functions $\mathrm{erf}(t)$, $t\,\mathrm{erf}(t)$ and $t^2\,\mathrm{erf}(t)$ generated by the code using the graphics application of your choice.

(b) Modify the code to plot any other special (ie not elementary) function of your choice.

(c) Measure the runtime, R, of the code for dt taking the values $1 \times 10^{-5}, 1 \times 10^{-6}, 1 \times 10^{-7}, 1 \times 10^{-8}$. How would you expect R to depend on dt? Plot your measurements in such a way as to make this clear (you should be able to obtain a straight line).

1.2 Solving a system of linear equations using the GSL library

Download the sample code worksheet1-Q1.2.tgz from the class website. It demonstrates how to use GSL to solve the 5×5 linear system

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{pmatrix} = \begin{pmatrix} A \\ 0 \\ 0 \\ 0 \\ B \end{pmatrix} \tag{1}$$

Questions

(a) Modify the sample code (or write your own code) to solve the corresponding $N \times N$ problem for $N = 10^3$, $N = 10^4$ and $N = 10^5$.

(b) For each value of N, plot x_n as a function of n. From these graphs, can you guess the solution of the linear system for general N (ie write a formula expressing x_n as a function of A, B, N and n)?

(c) How is this linear system related to the boundary value problem.

$$\frac{d^2u}{dx^2} = 0 \tag{2}$$

on the interval $[x_L, x_R]$ with the boundary conditions $u(x_L) = A$, $u(x_R) = B$?

1.3 Taylor's Theorem

This is just to get some familiarity with Taylor's Theorem.

Questions

(a) Write down Taylor's Theorem with the Lagrange form of the error.

(b) Write down the Taylor expansions in powers of h of the following functions up to and including terms of order h^2:

- $\sin(t + h)$
- $\sin\left(\frac{1}{2}(t + h)^2\right)$
- $\sin\left(\frac{1}{2}t^2 + \lambda h\right)$ where $\lambda \in \mathbb{R}$

(c) For the exponential function $v(t) = \mathrm{e}^{\lambda t}$, find explicitly the value of ξ in the remainder term of the first order Taylor expansion. Under what conditions can the remainder term be large?

2 Group work

2.1 Numerical Error Analysis

Download and unpack the tarball worksheet1-Q2.1.tgz from the class website. The code uses the simple Euler method to solve the equation used as an example in the notes:

$$\frac{d^2v}{dt^2} + 2\,t\frac{dv}{dt} - \alpha v = 0, \tag{3}$$

for the particular case of $\alpha = 0$, $v(0) = 0$, $\frac{dv}{dt}(0) = \frac{2}{\sqrt{\pi}}$, Eq. (3) has a simple exact solution:

$$v(t) = \mathrm{erf}(t) = \frac{2}{\sqrt{\pi}} \int_0^t e^{-s^2}\, ds, \tag{4}$$

Questions

(a) Write Eq. (3) as a 3-dimensional first order system:

$$\frac{d\mathbf{v}}{dt} = \mathbf{G}(\mathbf{v}), \tag{5}$$

where $\mathbf{v}(t) = (v^{(1)}(t), v^{(2)}(t), v^{(3)}(t))$.

(b) Write down the exact solution, $\mathbf{v}_{\mathrm{exact}}(t)$, of this first order system corresponding to the exact solution, Eq. (4), when $\alpha = 0$ (ie write down explicit formulae for the components of the vector $\mathbf{v}(t)$ as functions of time).

(c) From numerical explorations, or otherwise, describe how the solution changes when $\alpha \neq 0$. Plot some graphs.

(d) Returning to the case $\alpha = 0$. Let us denote the numerical solution produced by the code as $\mathbf{v}_{\mathrm{numerical}}(t)$. One reasonable measure of the global error in the numerical solution over the interval $[0, T]$ is

$$E(T) = \int_0^T \left|\mathbf{v}_{\mathrm{numerical}}(\tau) - \mathbf{v}_{\mathrm{exact}}(\tau)\right|\, d\tau. \tag{6}$$

Can you think of any others? We can approximate $E(T)$ by the Riemann sum

$$E(T) = \sum_i \left|\mathbf{v}_{\mathrm{numerical}}(t_i) - \mathbf{v}_{\mathrm{exact}}(t_i)\right|\, h. \tag{7}$$

Show *empirically* (ie from numerical measurements) that $E(T)$ is proportional to h as $h \to 0$.

(e) Modify the code to use the Improved Euler method and show empirically that the global error is then proportional to h^2 as $h \to 0$.

2.2 Runge-Kutta Methods

Consider the following initial value problem on the interval $[0, 1]$:

$$\begin{aligned} \frac{d^2v}{dt^2} - (1+\alpha v^2)\, v &= 0 \\ v(0) &= 0 \\ \frac{dv}{dt}(0) &= 1. \end{aligned} \tag{8}$$

The solution in the linear case, $\alpha = 0$, is

$$v(t) = \sinh(t). \tag{9}$$

Questions

1. Write down your favourite 3rd order Runge-Kutta algorithm. What is the global error?
2. Implement it and use it to solve the initial value problem (8) with $\alpha = 0$. Show empirically that the global error behaves as you expect as $h \to 0$.
3. Solve the nonlinear initial value problem (8) for several values of α in the range $0 < \alpha \leq 10$. Plot your results. Do you think they make sense?
4. An analytic solution is much harder to write down when $\alpha > 0$. Estimate the error using the two-step method and show empirically that the global error behaves as you expect in the nonlinear case as $h \to 0$.
5. Consider the nonlinear problem with $\alpha = 10$. Can you solve the initial value problem over the interval $0 < t < 2$?

2.3 Boundary Value Problems

Consider the boundary value problem related to Eq. (8):

$$\begin{aligned} \frac{d^2v}{dt^2} - (1+\alpha v^2)\, v &= 0 \\ v(0) &= 0 \\ v(1) &= 1. \end{aligned} \tag{10}$$

The solution in the linear case, $\alpha = 0$, is

$$v(t) = \frac{2\,\mathrm{e}\,\sinh(t)}{\mathrm{e}^2 - 1}. \tag{11}$$

Questions

1. Using a centred finite difference representation for the derivative, discretise the problem on a set of N equally spaced points. Show that the discrete problem is equivalent to a set of N linear equations. What is the accuracy of your approximation?
2. Use your linear solver from Question 1.2 to solve this set of linear equations numerically with $N = 10^2$, $N = 10^3$, $N = 10^4$ and $N = 10^5$. Do the resulting solutions look like the true solution, Eq. (11)? Measure the error and comment on how it varies as N is increased.
3. Explain why this approach will not work for the nonlinear problem, $\alpha > 0$.
4. Use your Runge-Kutta algorithm from Question 2.2 to solve the nonlinear problem with $\alpha = 10$ using the shooting method (shoot in the range $0.25 < \frac{dv}{dt}(0) < 1.25$). Plot your solution and compare it to the solution of the corresponding linear problem.