Mathematical Computing: Numerical Methods   2015

Lecturer: *D. J. Ivers*

Assignment 2 — Quadrature and Initial Value Problems for Systems of ODE's

Hand-written Questions 1 and 2 due 5pm Thursday 4th June.
Programming Questions 3 and 4 due 5pm Thursday 4th June.

Read the course messages for general information on assignments, the form your Assignment 2 file must take and how to submit it. This assignment is worth 8 marks.

1. The 2-point Gauss rule for the weight e^{-x} on the interval $[0, \infty]$ is of the form

$$\int_0^\infty f(x)e^{-x}\,dx \approx w_1 f(x_1) + w_2 f(x_2)\,.$$

(a)   Using the Gram-Schmidt procedure determine the orthogonal polynomials $\phi_0(x)$, $\phi_1(x)$ and $\phi_2(x)$ for the weight function $w(x) = e^{-x}$ in $0 \le x \le \infty$. Find also A_0, A_1, A_2, γ_0, γ_1. Suggestion: show

$$\int_0^\infty x^n e^{-x}\,dx = n!\,, \qquad n = 0, 1, 2, 3, \ldots\,.$$

(The integral on the left is actually the Gamma (or factorial) function $\Gamma(n+1)$. $\phi_n(x)$ is the n-degree Laguerre polynomial.)

(b)   Determine the nodes x_1 and x_2 for the 2-point weighted Gauss rule from $\phi_2(x)$.

(c)   Using the recurrence relation

$$\phi_{k+1}(x) - (a_k x + b_k)\phi_k(x) + c_k \phi_{k-1}(x) = 0$$

given in the notes show that the weights

$$w_k = -\frac{A_{n+1}\gamma_n}{A_n \phi_{n+1}(x_k)\phi_n'(x_k)}$$

can be expressed in the more useful form

$$w_k = \frac{A_n \gamma_{n-1}}{A_{n-1}\phi_{n-1}(x_k)\phi_n'(x_k)}\,.$$

Hence determine the weights w_1 and w_2 for the 2-point weighted Gauss rule.

2. Consider the initial value problem

$$\frac{dy}{dt} = f(t,y), \qquad y(0) = y_0.$$

(a) By expanding the exact solution $y = Y(t)$ of the initial value problem in a two term Taylor series with remainder about $t = t_{k+1}$, show that

$$Y_k = Y_{k+1} - hf(t_{k+1}, Y_{k+1}) + \tfrac{1}{2}Y''(\xi_k)h^2,$$

where $Y_k \equiv Y(t_k)$, etc., and ξ_k lies between t_k and t_{k+1}.

(b) By subtracting the equation derived in Part (a) from the backward-Euler method,

$$y_{k+1} = y_k + hf(t_{k+1}, y_{k+1}),$$

deduce that the global error e_k in the backward-Euler method satisfies

$$e_{k+1} = \frac{e_k}{1 - hJ} - \frac{Y''(\xi_k)h^2}{2(1 - hJ)},$$

where $J = f_y(t_{k+1}, \eta_{k+1})$ and η_{k+1} lies between y_{k+1} and Y_{k+1}.

(c) Deduce from Part (b) that the backward-Euler method is stable, when applied to well-conditioned problems, if $h > 0$ or $h < 2/J < 0$. Thus the step-size $h > 0$ in the backward-Euler method is unrestricted by stability considerations and can be chosen for accuracy.

3. Attached is a listing of the file `ass2.inc` which contains an incomplete main program implementing the classical fourth-order Runge-Kutta for solving the second-order initial value problem

$$My'' + ry' + Mg = 0\,, \qquad y(0) = H\,, \quad y'(0) = 0\,,$$

for an object of mass M dropped from a vertical height H in a uniform gravitational field g and subject to an air resistance proportional to the velocity. Assume $M = 10\,\text{kg}$, $r = 0$, $g = 10\,\text{m}^2\,\text{s}^{-1}$ and $H = 10\,\text{m}$. In `ass2.inc` a question mark `?` indicates a missing single character, three horizontal dots `...` indicates a missing part or the missing whole of a line and three vertical dots indicates a missing block (two or more lines) of code. Save the file to your directory and complete the program to have the following features:

(a) The problem parameters (`mass` (for M), `r` and `g` in Question 3; `mu` and `mut` in Question 4) are input from a file called `parameters.dat` using a namelist `parameters` and echoed to the screen. Save the file `parameters.dat` to your directory.

(b) The arrays `y`, `yrk4`, `k1`, `k2`, `k3`, `k4` are declared and dimensioned in the main program.

(c) The initial time `t0`, the final time `tn`, the number of steps `n`, the output frequency `nprint` and the vector $\mathbf{y}_0$ of initial values are input from a file using a namelist `run_data` and echoed to the screen. Use the array `y` for the vector $\mathbf{y}_0$ of initial values. The name of the data file is input from the workstation with a prompt.

(d) The values of `t` and `y` are written into a file with appropriate headers. An implied do-loop is not used for `y`. The name of the output file is input from the workstation with a prompt.

(e) The step-size `h` is set by `t0`, `tn` and `n`.

(f) Values of `t` and `y` are printed every `nprint` steps with format descriptors `F14.5` and `E14.5`, respectively.

(g) The first-order system of ode's is given by the array-valued internal function `f`. Local arrays `y` and `f_result` are declared and dimensioned in `f`.

(h) The fourth-order Runge-Kutta subroutine is `rk4` from Set 5.

4. Consider the following Earth-Moon-spaceship problem,

$$x'' = 2y' + x - \frac{\tilde{\mu}(x + \mu)}{r_1^3} - \frac{\mu(x - \tilde{\mu})}{r_2^3},$$

$$y'' = -2x' + y - \frac{\tilde{\mu}y}{r_1^3} - \frac{\mu y}{r_2^3},$$

where $\tilde{\mu} = 1 - \mu$, $r_1^2 = (x + \mu)^2 + y^2$ and $r_2^2 = (x - \tilde{\mu})^2 + y^2$. The coordinates of the spaceship are (x, y) in a reference frame rotating with the Earth and the Moon, which are at $(-\mu, 0)$ and $(\tilde{\mu}, 0)$, respectively. The equations have been scaled so that distance is measured in units of the Earth-Moon distance R, time in units of Ω^{-1}, where Ω is the angular speed of the Moon about the Earth and velocity in units of $R\Omega$. Since the mass of the spaceship is negligible compared to the masses of the Earth and Moon, the Earth-Moon-spaceship problem is a case of the restricted three-body problem.

Modify your program from Question 3 to solve the Earth-Moon-spaceship problem. Use the following initial values of the dependent variables

$$x(0) = 0.994, \qquad y(0) = 0, \qquad x'(0) = 0, \qquad y'(0) = -2.0015851,$$

for $\mu = 0.012277471$. Take `t0`=0, `tn`=17.5, `n`=20000 and `nprint`=50.

(a)   Show numerically that the orbit is periodic and find the period as accurately as possible.

(b)   Find the minimum radius from the Moon to the orbit. Use a block-if in the t_loop to determine the latest minimum radius `r2_min` and the corresponding time `t_min`, position and velocity `y_min`. Output the results to the screen with appropriate headers after completing the t_loop. From your output file (output t, x, y, x', y', r_2) determine the time(s), position(s) and velocity(ies) of any other points of the orbit, where the minimum radius occurs.

(c)   Use funplot to plot the orbit.

Read the course messages for details on what to hand in.

```fortran
program rk4sysmain
!-------------------------------------------------------------
! This program solves the initial value problem for a system
! of first-order differential equations using the classical
! fourth-order Runge-Kutta method.
!-------------------------------------------------------------
! Declare problem size:
integer, parameter :: m=?

! Declare program variables:
real :: mass,...
integer :: n, ...
real :: t0, ...
real, dimension(m) :: y, ...
character(len=20) :: datafile, ??????
namelist /??????????/ mass,...
???????? /run_data/ t0,...,y

!...Open and enter parameters from file parameters.dat:
open (unit=7, file='parameters.dat', status='old')
read (7,nml=parameters)
close(7)

!...Echo parameters to terminal:
write (*,nml=parameters)

!...Name, open and enter run_data from data_file:
write (*,*) ' Enter run_data file name:'
read (*,10) ????????
10 format (a)
open (????=7, file=datafile, status='old')
read (7,nml=...)
close(7)

!...Echo run_data to terminal:
write (*,???=run_data)

! Name, open and head output file:
write (*,*) ' Enter output file name:'
read (*,10) output
open (unit=8, file=??????, status='unknown')
write (8,30)
30 format('   t          y            y'' ')  !Q1 (adjust spacing if needed)
!30 format('  t         x      ...               !Q2

! Initialise values for DO-loop (y initialised directly by input):
t = ...
h = ...

! Initialise min_r2 for Q2 only:
! r2_min = ...  !Q2
t_loop: do j= 1, ?
   ! 4th order Runge-Kutta subroutine:
   call rk4
   y = ????
   t = ...
```

```fortran
   ! Print solutions every nprint steps:
   if ( mod(j,nprint)==0 ) then
!      r2 = ...   !Q2
!       write (8,40) t, ..., r2   !Q2
      write (8,40) t, ...
40    format (?????, ??????)
   endif

   ! The following code is for Question 2 only:
   !r2 = ...
   !Calculate the minimum of r2:
   !if (r2_min > r2) then
   !   r2_min= ...
   !   .
   !   .
   !endif

enddo t_loop
! The following ... is for Question 2 only:
! Output the minimum of r2 and associated values of t,y:
   !   .
   !   .
   !   .

stop
????????
!-------------------------------------------
function f(t,y) result(f_result)
real, intent(in):: t
real, dimension(m), intent(in):: y
real, dimension(m) :: f_result

f_result(1) = ...
   !   .
   !   .
   !   .

end ???????? ?
!----------------------------------------------------------------
subroutine rk4
   ! Purpose:  To implement the classical fourth-order Runge-Kutta
   ! method for the system of M first-order differential equations
   ! y'=f(t,y) over one interval of width h.  Thus subroutine rk4
   ! approximates y(t+h) with yrk4, given y=y(t).
k1 = h*f(t,y)
k2 = h*f(t + h/2.,y + k1/2.)
k3 = h*f(t + h/2.,y + k2/2.)
k4 = h*f(t+h,y+k3)
yrk4 = y + (k1 + 2.*k2 + 2.*k3 + k4)/6.
return
end subroutine rk4
!----------------------------------------------------------------
end ...
```