PHYS 410 Homework 2

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Introduction

In this homework assignment, the fourth-order Runge-Kutta method for computing numerical solutions of ODEs is explored. This is done in stages, culminating in creating a MATLAB function that numerically integrates an ODE using an algorithm that automatically varies the step size of the integrator in order to achieve a relative error tolerance.

First, a function rk4step is written that computes a single fourth-order Runge-Kutta step for a system of coupled first-order ODEs, returning the approximate values of the dependent variables after a defined time step. The function rk4step is then used in the function rk4 which computes the solution of an initial value problem over a range of values for the independent variable, done by taking multiple fourth-order Runge-Kutta steps in a loop. Lastly, the function rk4ad is written which finds the numerical solution of an initial value problem by comparing the results of fourth-order Runge-Kutta steps of different sizes and then varying the step size as until the error in the approximation is below a specified relative tolerance.

Review of Theory
Casting systems of ODEs in first-order form
The fourth-order Runge-Kutta step
Numerical Approach
Consecutive fourth-order Runge-Kutta steps
Adaptive step sizing
Implementation
ODE test functions
Results
rk4step.m Output
rk4.m Output
rk4ad.m Output

Conclusions

Appendix A - rk4step.m Code

```
‰ Problem 1 − Single Fourth Order Runge-Kutta Step
  % Function that computes a single fourth order Runge-Kutta Step.
  %
4
  % Inputs
  %
                   Function handle for right hand sides of ODEs (returns
           fcn:
  %
                   length-n column vector).
  %
           t0:
                   Initial value of independent variable.
  %
                   Time step.
           dt:
  %
           y0:
                   Initial values (length-n column vector).
10
  %
11
  % Output
12
                   Final values (length—n column vector)
13
           yout:
   function yout = rk4step(fcn, t0, dt, y0)
14
      % Compute terms in RK step
15
       f0 = fcn(t0, y0);
16
       f1 = fcn(t0 + dt/2, y0 + (dt/2)*f0);
17
       f2 = fcn(t0 + dt/2, y0 + (dt/2)*f1);
18
       f3 = fcn(t0 + dt, y0 + dt*f2);
       % Add terms to compute full RK step
20
       yout = y0 + (dt/6)*(f0 + 2*f1 + 2*f2 + f3);
21
  _{
m end}
22
```

Appendix B - trk4step.m Code

```
% Problem 1 − Test Script
2
  close all; clear; clc;
3
  format long;
5
  % Function that computes right hand sides of ODEs for simple harmonic
7
  % oscillator with unit angular frequency. For use in rk4step, rk4, and
      rk4ad.
  %
  % Governing DE:
  % Canonical first order dependent variables:
                                                     x1 = x, x2 = x'
  % System of Equations:
                                                     x1' = x2, x2' = -x1
13
  % Inputs
  %
                   Independent variable at current time-step
           t:
  %
                   Dependent variables at current time-step (length-n column
16
           x:
  %
                   vector).
17
  %
  % Outputs
19
                  Computes the derivatives of x1 and x2 at the current
           dxdt:
20
                  time-step (length-n column vector).
21
  function dxdt = fcn_sho(t, x)
       dxdt = zeros(2,1);
23
       dxdt(1) = x(2);
24
       dxdt(2) = -x(1);
25
26
  end
27
  % Function parameters for exact solution of x(t) = \sin(t)
28
  x0 = [0; 1];
                   % Initial conditions
                   \% Initial time
  t0 = 0;
  % Vector of linearly increasing time-step lengths
  dt = linspace(0.01, 0.3, 1000);
32
33
  % Run Runge-Kutta step at various time steps
  xout = zeros(2, length(dt));
35
  for i = 1: length(dt)
36
       xout(:,i) = rk4step(@fcn_sho, t0, dt(i), x0);
37
38
39
  % Calculate the error at each time step length using the known exact
40
      solution
   errors = abs(xout(1,:) - sin(dt));
41
42
  % Plot error as a function of dt and compare to C*t^5
43
  hold on;
  plot(dt, errors, "Color", 'r', "LineWidth", 3);
  C = 8.3e - 3;
  plot(dt, C*dt.^5, "--", "Color", 'b', "LineWidth", 3);
   title ("Magnitude of error vs. time step length dt shown to scale as dt^5");
  xlabel("Time step length dt");
  ylabel("Magnitude of error");
  legend(["Error", "C * t^5"], 'location', 'best');
  ax = gca;
  ax.FontSize = 12;
```

Appendix C - rk4.m Code

```
% Problem 2 - Runge-Kutta System of ODEs Integrator
  % Function that numerically computes the solution to a system of ODEs
3
  % over a given period of time using a fourth-order Runge-Kutta method.
  % Inputs
  %
           fcn:
                    Function handle for right hand sides of ODEs (returns
  %
                    length—n column vector)
  %
                    Vector of output times (length nout).
           tspan:
  %
                    Initial values (length-n column vector).
           v0:
10
  %
11
  % Outputs
12
  %
                    Vector of output times.
13
           tout:
  %
           yout:
                    Output values (nout x n array. The ith column of yout
14
                    contains the nout values of the ith dependent variable).
15
   function [tout yout] = rk4(fcn, tspan, y0)
16
       % Number of equations in ODE system
17
       n = \max(size(y0));
18
       % Number of time-steps
       nout = max(size(tspan));
20
21
       % Initialize array for output values
22
       yout = zeros(nout, n);
23
       yout(1,:) = y0.';
24
25
       % Integrate ODE
26
       for i = 2:nout
           \% Step size for the current step
28
           dt \,=\, tspan\left(\,i\,\right) \,-\, tspan\left(\,i\,{-}1\right);
29
           \% Compute the values of the dependent variables at the next step
30
           yout(i,:) = rk4step(fcn, tspan(i-1), dt, yout(i-1,:).').';
31
       end
32
33
       % Generate array of output values
34
       tout = tspan;
  end
36
```

Appendix D - trk4_sho.m Code

```
% Problem 2 - Test Script - Simple Harmonic Oscillator
2
   close all; clear; clc;
3
   format long;
5
  % Function that computes right hand sides of ODEs for simple harmonic
7
  % oscillator with unit angular frequency. For use in rk4step, rk4, and
      rk4ad.
  %
  % Governing DE:
  % Canonical first order dependent variables:
                                                          x1 = x, x2 = x
  % System of Equations:
12
                                                          x1' = x2, x2' = -x1
13
  % Inputs
  %
                     Independent variable at current time-step
            t:
  %
                     Dependent variables at current time-step (length-n column
16
            x:
  %
                     vector).
17
  %
  % Outputs
19
                    Computes the derivatives of x1 and x2 at the current
            dxdt:
20
                    time-step (length-n column vector).
21
   function dxdt = fcn_sho(t, x)
       dxdt = zeros(2,1);
23
       dxdt(1) = x(2);
24
       dxdt(2) = -x(1);
25
26
   end
27
  % Function parameters for exact solution of x(t) = \sin(t)
28
                              \% Initial conditions
   x0 = [0; 1];
                              \% Start and end times
   t0 = 0; tf = 3*pi;
31
  % Vector of output times for each discretization level
32
   tspan6 = linspace(t0, tf, 2^6 + 1);
   tspan7 = linspace(t0, tf, 2^7 + 1);
   tspan8 = linspace(t0, tf, 2^8 + 1);
35
36
  % Compute ODE numerical solution at each discretization level
   [tout6 	ext{ xout6}] = rk4(@fcn_sho, tspan6, x0);
    [tout7 	ext{ xout7}] = rk4(@fcn_sho, tspan7, x0);
39
   [tout8 xout8] = rk4(@fcn_sho, tspan8, x0);
40
  % Plot the solutions at each discretization level
   fig1 = figure(1);
43
  hold on
44
   plot(tout6, xout6(:,1), "LineWidth", 2);
   \begin{array}{ll} \textbf{plot} \, \big( \, \textbf{tout7} \, \, , \, \, \, \textbf{xout7} \, \big( \, \vdots \, , 1 \, \big) \, \, , \, \, \, \text{"LineWidth"} \, , \, \, \, 2 \, \big) \, ; \end{array}
   plot(tout8, xout8(:,1), "LineWidth", 2);
47
   title ("Numerical solutions to SHO ODE at various discretization levels");
   xlabel("Independent Variable t");
   ylabel("Dependent Variable x");
   legend(["1 = 6", "1 = 7", "1 = 8"], 'location', 'best');
51
   ax = gca;
52
   ax.FontSize = 12;
  % Compute the errors at each time step for each discretization level
```

```
errors6 = xout6(:,1) - sin(tout6).;
   errors7 = xout7(:,1) - sin(tout7).';
   errors8 = xout8(:,1) - sin(tout8).';
   % Plot the scaled errors for each discretization level
60
   fig2 = figure(2);
   hold on
   plot(tout6, errors6, "LineWidth", 2);
   plot(tout7, 2^4*errors7, "LineWidth", 2);
plot(tout8, 4^4*errors8, "LineWidth", 2);
   title({"Scaled errors of numerical solutions to SHO ODE at ", ... "various discretization levels"});
67
68
   xlabel("Independent Variable t");
   ylabel("Scaled error");
legend(["error @ l=6", "2^4 * error @ l=7", "4^4 * error @ l=8"], ...
'location', 'best');
70
71
72
  ax = gca;
ax.FontSize = 12;
```

Appendix E - trk4_vdp.m Code

```
‰ Problem 2 − Test Script − Van der Pol oscillator
2
  close all; clear; clc;
3
  format long;
5
  % Function that computes right hand sides of ODEs for Van der Pol
7
  % Oscillator. Following Tsatsos: https://arxiv.org/pdf/0803.1658
  % Governing DE: x'' = -x - a(x^2 - 1)x'
10
  \% Canonical first order dependent variables: x1 = x, x2 = x
  % System of Equations:
           x1' = x2
13
  %
           x2' = -x1 - a(x1^2 - 1)*x2
14
  %
  % Inputs
  %
                   Independent variable at current time-step
17
           t:
  %
                    Dependent variables at current time-step (length-n column
           \mathbf{x}:
18
  %
                    vector).
19
20
  % Outputs
21
           dxdt:
                  Computes the derivatives of x1 and x2 at the current
22
  %
                   time-step (length-n column vector).
  function dxdt = fcn_vdp(t, x)
24
       global a:
25
       dxdt = ones(2,1);
26
       dxdt(1) = x(2);
27
       dxdt(2) = -x(1) - a*(x(1)^2 - 1)*x(2);
28
  end
29
30
  \% Function parameters
                       % Initial conditions
  x0 = [0; -6];
  t0 = 0; tf = 100;
                       % Start and end times
33
  global a; a = 5;
                       % Adjustable parameter
34
  % Discretization level
36
  level = 12;
37
  tspan = linspace(t0, tf, 2^level + 1);
  % Compute ODE numerical solution
40
  [tout xout] = rk4(@fcn_vdp, tspan, x0);
41
  % Plot position vs time
43
  fig1 = figure(1);
44
  plot(tout, xout(:,1), "LineWidth", 2)
   title ("Numerical solution of Van der Pol oscillator ODE - Position x vs.
      Time t");
  xlabel("Independent Variable - Time t");
47
  ylabel("Dependent Variable - Position x");
  ax = gca;
  ax.FontSize = 12;
50
51
  % Plot phase space evolution
  fig2 = figure(2);
  plot (xout (:,1), xout (:,2), "LineWidth", 2)
  title ({" Phase space evolution of Van der Pol oscillator ODE", ...
```

```
"Velocity dx/dt vs. Position x"}); xlabel("Position x"); ylabel("Velocity dx/dt"); ax = gca; ax. FontSize = 12;
```

Appendix F - rk4ad.m Code

```
M Problem 3 - Adaptive Fourth Order Runge-Kutta System of ODEs Integrator
2
  % Function that numerically computes the solution to a system of ODEs
3
  % over a given period of time using a fourth-order Runge-Kutta method
  % with adaptive steps sizes to ensure a relative tolerance is reached.
  %
  % Inputs
  %
                   Function handle for right hand sides of ODEs (returns
           fcn:
  %
                   length-n column vector)
                   Vector of output times (length nout vector).
           tspan:
10
  %
           reltol: Relative tolerance parameter.
11
  %
                   Initial values (length-n column vector).
13
  % Outputs
14
  %
                   Output times (length-nout column vector, elements
           tout:
15
  %
                   identical to tspan).
  %
                   Output values (nout x n array. The ith column of yout
17
           yout:
  %
                   contains the nout values of the ith dependent variable).
18
  function [tout yout] = rk4ad(fcn, tspan, reltol, y0)
      % Number of equations in ODE system
20
       n = \max(size(y0));
21
      % Number of time-steps
22
       nout = max(size(tspan));
      % Lower bound on step size
24
       floor = 1.0e-4;
25
26
      % Initialize array for output values
       yout = zeros(nout, n);
28
       yout(1,:) = y0.';
29
30
      % Integrate ODE
31
       for i = 2: nout
32
           % Compute coarse rk4step arguments
33
           tprev = tspan(i-1);
           yprev = yout(i-1,:).;
           dt = tspan(i) - tspan(i-1);
36
37
           % Compute fine and coarse approximations for y(tprev + dt)
           yc = rk4step(fcn, tprev, dt, yprev);
39
           if dt/2 < floor
40
               % If fine step is lower than floor, cannot narrow down any
41
                   further
               yout(i,:) = yc.';
42
               continue;
43
           end
44
           yhalf = rk4step(fcn, tprev, dt/2, yprev);
           yf = rk4step(fcn, tprev + dt/2, dt/2, yhalf);
46
47
           % Check if error meets relative tolerance parameter
           if abs((yc - yf)/yf) < reltol
               yout(i,:) = yf.;
50
               continue;
51
           else
52
               % Iteratively compute yf at repeatedly halved dt sizes
               % until reltol is met or floor is reached
54
               i = 2;
55
```

```
while dt/(2\hat{j}) > floor \% Decrease step size by half each
56
                    iteration\\
                    yc = yf;
57
                    yf = yprev;
58
                    for k = 0:2^j - 1\% Number of steps to get to tprev + dt
59
                         yf = rk4step(fcn, tprev + k*dt/(2^j), dt/(2^j), yf);
                    end
61
62
                     if abs((yc - yf)/yf) < reltol
63
                         break;
                    end
65
66
                    j = j + 1;
67
                end
                yout(i,:) = yf.';
69
           end
70
       end
71
72
       \% Generate array of output values
73
       tout = tspan;
74
  end
75
```

Appendix G - trk4ad_sho.m Code

```
% Problem 3 - Test Script - Simple Harmonic Oscillator
2
   close all; clear; clc;
3
  format long;
5
  % Function that computes right hand sides of ODEs for simple harmonic
  % oscillator with unit angular frequency. For use in rk4step, rk4, and
      rk4ad.
  %
  % Governing DE:
  % Canonical first order dependent variables:
                                                      x1 = x, x2 = x'
  % System of Equations:
                                                      x1' = x2, x2' = -x1
13
  % Inputs
  %
                    Independent variable at current time-step
           t:
  %
                    Dependent variables at current time-step (length-n column
16
           x:
  %
                    vector).
17
  %
  % Outputs
19
                   Computes the derivatives of x1 and x2 at the current
           dxdt:
20
                   time-step (length-n column vector).
21
  function dxdt = fcn_sho(t, x)
       dxdt = zeros(2,1);
23
       dxdt(1) = x(2);
24
       dxdt(2) = -x(1);
25
26
  end
27
  % Function parameters for exact solution of x(t) = \sin(t)
28
                                              % Initial conditions
  x0 = [0; 1];
   tspan = linspace(0.0, 3.0 * pi, 65);
                                             % Vector of output times
31
  % Compute ODE numerical solution at each relative tolerance
32
   [tout5 xout5] = rk4ad(@fcn_sho, tspan, 1.0e-5, x0);
33
    tout7 xout7] = rk4ad(@fcn_sho, tspan, 1.0e-7, x0);
    tout9 xout9] = rk4ad(@fcn_sho, tspan, 1.0e-9, x0);
35
   [tout11 \ xout11] = rk4ad(@fcn_sho, tspan, 1.0e-11, x0);
36
37
  % Plot the solutions at each relative tolerance
38
  fig1 = figure(1);
39
  hold on
40
   plot(tout5, xout5(:,1), "LineWidth", 2);
   plot(tout7, xout7(:,1), "LineWidth", 2);
plot(tout9, xout9(:,1), "LineWidth", 2);
43
   plot (tout11, xout11(:,1), "LineWidth", 2);
   title ("Numerical solutions to SHO ODE from rk4ad at various relative
      tolerances");
   xlabel("Independent Variable t");
46
   ylabel("Dependent Variable x");
   legend(["reltol = 1.0e-5", "reltol = 1.0e-7", "reltol = 1.0e-9", ...]
           "reltol = 1.0e-11"], 'location', 'best');
49
  ax = gca;
50
  ax.FontSize = 12;
51
  % Compute the errors at each time step for each discretization level
53
  errors5 = xout5(:,1) - sin(tout5).;
```

```
errors7 = xout7(:,1) - sin(tout7).;
   errors 9 = \text{xout} 9 (:,1) - \sin(\text{tout} 9).';
   errors11 = xout11(:,1) - sin(tout11).';
   % Plot the errors for each relative tolerance
59
   fig2 = figure(2);
   hold on
   plot(tout5, errors5, "LineWidth", 2);
plot(tout7, errors7, "LineWidth", 2);
plot(tout9, errors9, "LineWidth", 2);
   plot(tout11, errors11, "--", "LineWidth", 2);
   grid on
66
   title ({" Errors of numerical solutions to SHO ODE at ", \dots
67
            "various rk4ad relative tolerances"});
   xlabel("Independent Variable t");
ylabel("Error");
69
70
   legend (["reltol = 1.0e-5", "reltol = 1.0e-7", "reltol = 1.0e-9", ... "reltol = 1.0e-11"], 'location', 'best');
71
   ax = gca;
73
ax.FontSize = 12;
```

Appendix H - trk4ad_vdp.m Code

```
‰ Problem 3 − Test Script − Van der Pol oscillator
   close all; clear; clc;
3
  format long;
5
  % Function that computes right hand sides of ODEs for Van der Pol
7
  % Oscillator. Following Tsatsos: https://arxiv.org/pdf/0803.1658
  % Governing DE: x'' = -x - a(x^2 - 1)x'
  \% Canonical first order dependent variables: x1 = x, x2 = x
  % System of Equations:
           x1' = x2
13
  %
            x2' = -x1 - a(x1^2 - 1)*x2
14
  %
  % Inputs
  %
                     Independent variable at current time-step
17
            t:
  %
                     Dependent variables at current time-step (length-n column
            \mathbf{x}:
18
  %
                     vector).
19
20
  % Outputs
                    Computes the derivatives of x1 and x2 at the current
            dxdt:
22
  %
                    time-step (length-n column vector).
   function dxdt = fcn_vdp(t, x)
24
       global a:
25
       dxdt = ones(2,1);
26
       dxdt(1) = x(2);
27
       dxdt(2) = -x(1) - a*(x(1)^2 - 1)*x(2);
28
29
30
  % Function parameters
                                           % Initial conditions
  x0 = [0; -6];
   tspan = linspace(0.0, 100, 4097);
                                           % Vector of output times
33
   global a; a = 5;
                                           % Adjustable parameter
   reltol = 1.0e-10;
                                           % Relative tolerance
36
  % Compute ODE numerical solution
37
   [tout xout] = rk4ad(@fcn_vdp, tspan, reltol, x0);
39
  % Plot position vs time
40
  fig1 = figure(1);
41
   plot(tout, xout(:,1), "LineWidth", 2, "Color", 'm')
   title ({" Numerical solution of Van der Pol oscillator ODE using rk4ad", ...
43
          "Position x vs. Time t, Relative tolerance = 1.0e-10"});
44
   xlabel("Independent Variable - Time t");
   ylabel("Dependent Variable - Position x");
  ax = gca;
47
  ax.FontSize = 12;
48
  % Plot phase space evolution
   fig2 = figure(2);
   \operatorname{plot}\left(\operatorname{xout}\left(:,1\right),\ \operatorname{xout}\left(:,2\right),\ \operatorname{"LineWidth"},\ 2,\ \operatorname{"Color"},\ \operatorname{'m'}\right)
   title ({"Phase space evolution of Van der Pol oscillator ODE using rk4ad",
          "Velocity dx/dt vs. Position x, Relative tolerance = 1.0e-10"});
54
  xlabel("Position x");
```

```
ylabel("Velocity dx/dt");
ax = gca;
ax. FontSize = 12;
```