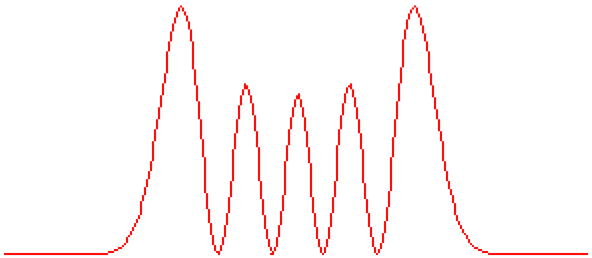
EP547 Computational Methods in QM

Topic 9

Ordinary Differential Equations



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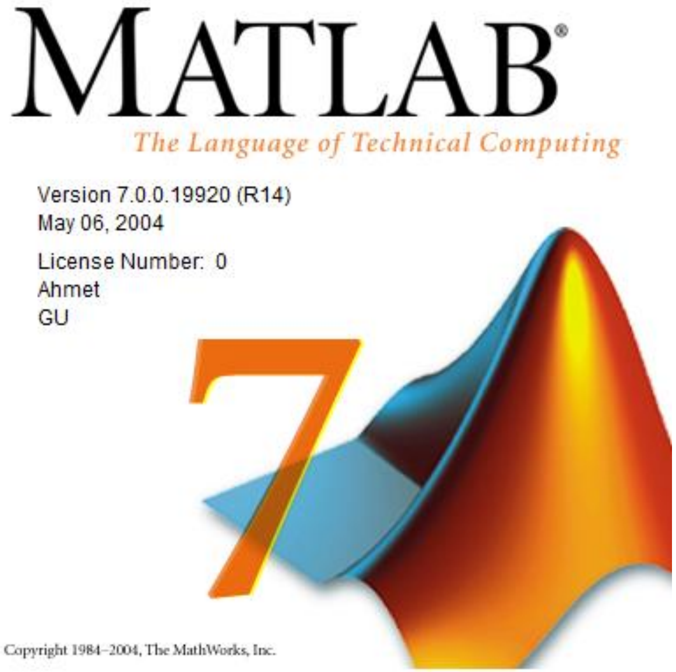


Introduction

- The numerical solution of differential equations is a very large subject spanning many types of problems and solutions.

- In this Lecture, we will consider the solutions of first and second order Differential Equations (DE) by using:

  - Euler Methods
  - Runge-Kutta Methods

Euler Methods

Simple Euler Method

Consider the following first order initial value problem:

$$\frac{dy}{dx} = f(x, y) \ ; \quad y_0 = y(x_0)$$

Solution can be obtained iteratively as follows:

$$y_{i+1} = y_i + f(x_i, y_i)h \qquad i = 0, 1, 2, \cdots, n$$

where

$$h = \frac{x_{max} - x_0}{n} \qquad i = 0, 1, 2, \cdots$$

and *n* is the number of points.

Example 1

Given an initial value problem:

$$y' = -xy \ ; \quad y(0) = 2$$

Find the numerical solution via Simple Euler method for the range 0<= x <=1 and n = 10 points.

Compare your results with the analytical solution:

$$y = 2e^{-x^2/2}$$

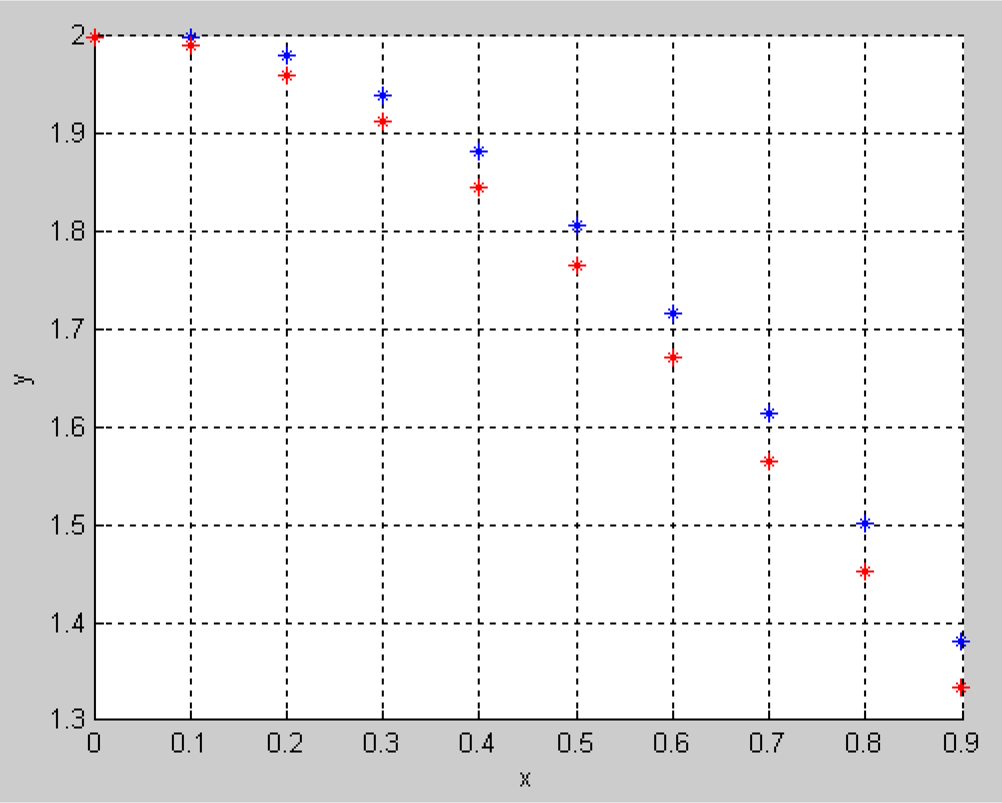
Solution 1

```
>> edit SimpleEuler.m
```

```
function SimpleEuler()
  hold on; grid on;
  x0=0;   y0=2;   xm=1;
  n=10; % number of points
  h=(xm-x0)/n;
  x(1)=x0;  y(1)= y0;

  for i=1:n-1
      y(i+1) = y(i) + f(x(i),y(i))*h;
      x(i+1) = x(i) + h;
      fprintf('%f  %f\n',x(i),y(i));
  end
  plot(x,y,'b*')
  plot(x,2*exp(-0.5*x.^2),'r*')
  xlabel('x')
  ylabel('y')
end

function z = f(x,y)
  z = -x*y;
end
```

Solution 1

```
>> SimpleEuler

0.000000  2.000000
0.100000  2.000000
0.200000  1.980000
0.300000  1.940400
0.400000  1.882188
0.500000  1.806900
0.600000  1.716555
0.700000  1.613562
0.800000  1.500613
```



Runge-Kutta Methods

Second Order

$$\frac{dy}{dx} = f(x, y) \;\; ; \quad y_0 = y(x_0)$$

$$\boxed{\begin{aligned} k_1 &= f(x_i, y_i) \\ k_2 &= f(x_i + h, y_i + k_1 h) \\ y_{i+1} &= y_i + \frac{h}{2}(k_1 + k_2) \end{aligned}}$$

Runge-Kutta Methods

Forth Order

$$\frac{dy}{dx} = f(x,y) \;;\quad y_0 = y(x_0)$$

$$\boxed{\begin{aligned}
k_1 &= f(x_i, y_i) \\
k_2 &= f(x_i + \frac{h}{2}, y_i + \frac{k_1 h}{2}) \\
k_3 &= f(x_i + \frac{h}{2}, y_i + \frac{k_2 h}{2}) \\
k_4 &= f(x_i + \frac{h}{2}, y_i + k_3 h) \\
y_{i+1} &= y_i + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4)
\end{aligned}}$$

Comparison

$$\frac{dy}{dx} = f(x, y) \; ; \quad y_0 = y(x_0)$$

Method	Order of error at each iteration
Simple-Euler	h
RK2	h^3
RK4	h^5

Second Order DEs

A 2nd order DE can be written as two first order DEs:

$$y'' = \frac{d^2y}{dx^2} = f(x,y) \; ; \quad y_0 = y(x_0), \quad y'_0 = y'(x_0)$$

Iterative solutions via Simple-Euler method are:

$$\boxed{\begin{array}{ll} \dfrac{du}{dx} = f(x,y) & \dfrac{dy}{dx} = u \\ u_{i+1} = u_i + f(x_i, y_i)h & y_{i+1} = y_i + u_i h \end{array}}$$

Iterative solutions via Euler-Cromer method are:

$$\boxed{\begin{array}{ll} \dfrac{du}{dx} = f(x,y) & \dfrac{dy}{dx} = u \\ u_{i+1} = u_i + f(x_i, y_i)h & y_{i+1} = y_i + u_{i+1} h \end{array}}$$

Example 2

Consider a body in free-fall (g = 9.8 m/s^2)

$$y'' = \frac{d^2 y}{dt^2} = -g \;\; ; \quad y(0) = 25\,\mathrm{m} \quad y'(0) = v = 0$$

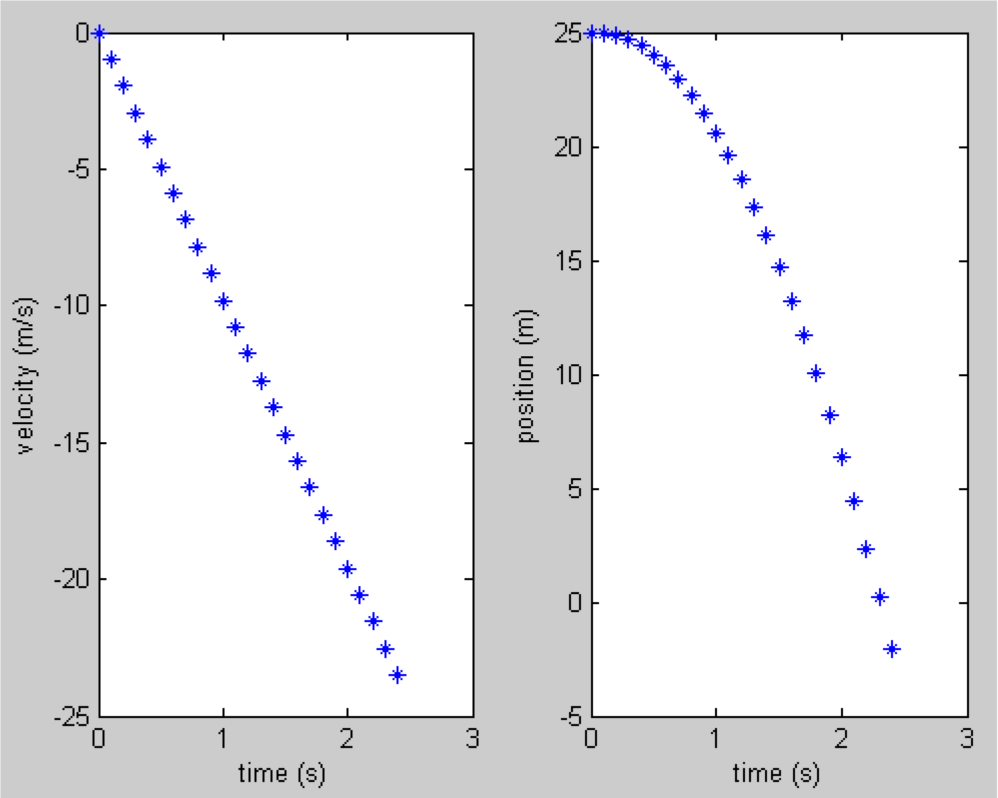
Find the numerical solution via Simple Euler method for the range 0<= y <=25 m and dt = 0.1 s.

Solution 2

```
>> edit FreeFall.m
```

```
function FreeFall()
  t(1)=0; u(1)=0; y(1)=25;
  i = 1; dt= 0.1;
  while y>0
      u(i+1) = u(i) - 9.8*dt;
      y(i+1) = y(i) + u(i)*dt;
      t(i+1) = t(i) + dt;
      fprintf('%f  %f %f\n',t(i), u(i), y(i));
      i = i+1;
  end
  subplot(1,2,1);
    plot(t,u,'b*')
    xlabel('time (s)')
    ylabel('velocity (m/s)')
  subplot(1,2,2);
    plot(t,y,'b*')
    xlabel('time (s)')
    ylabel('position (m)')
end
```

Solution 2



Example 3

Simple Pendulum:

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\theta \;\; ; \quad \theta(0) = 0.2$$

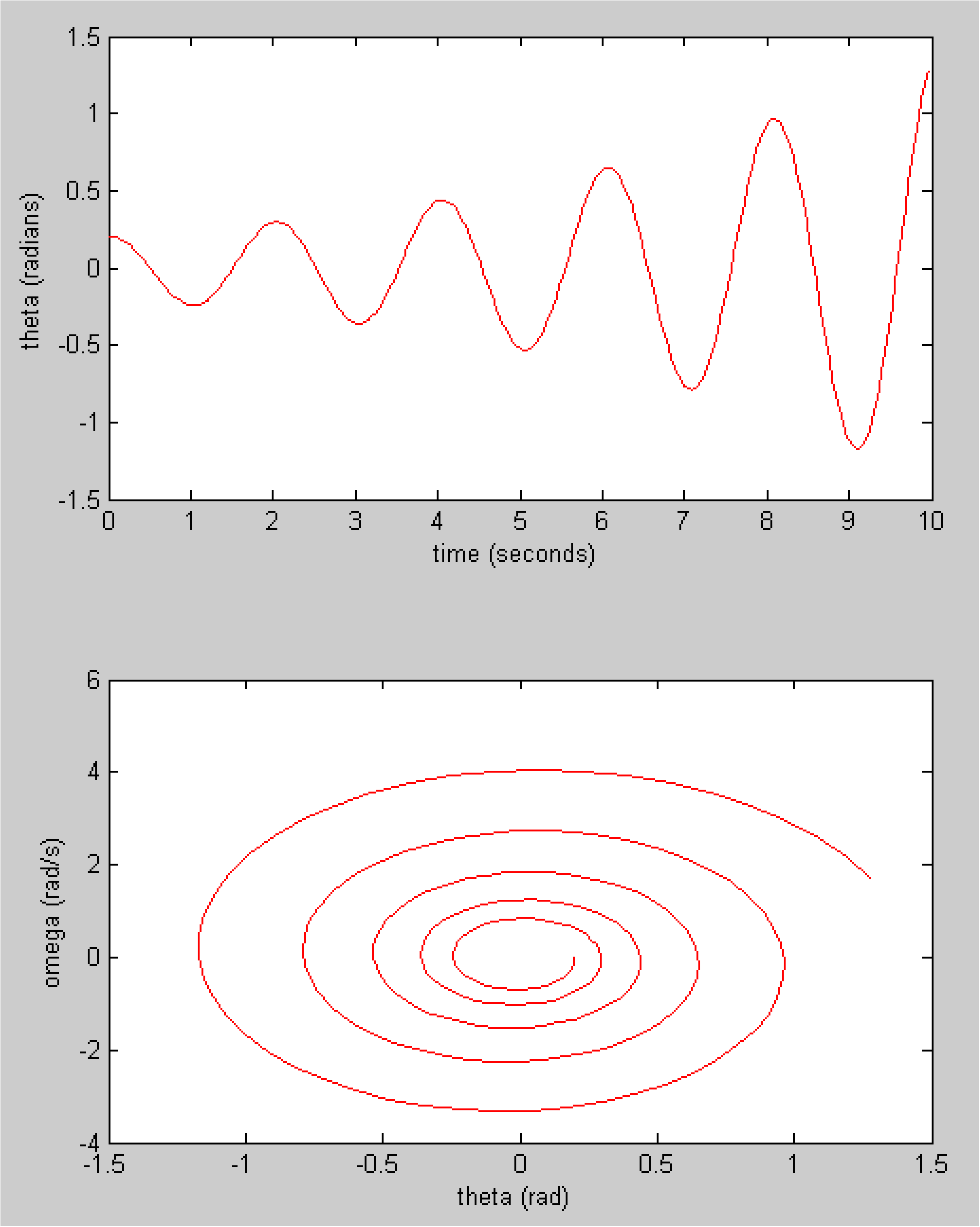
Find the numerical solution via Simple Euler and Euler-Cromer methods for dt = 0.04 s, L=1 m and n = 250 points.

Solution 3

```
>> edit pendulum1.m
```

```
L = 1;      % length of the pendulum in meters
g = 9.8;    % acceleration due to gravity
n = 250;    % Discretize time into 250 intervals
dt = 0.04;  % time step in seconds
omega = zeros(n,1);
theta = zeros(n,1);
t     = zeros(n,1);
theta(1) = 0.2;

for i = 1:n-1
   omega(i+1) = omega(i) - (g/L)*theta(i)*dt;
   theta(i+1) = theta(i) + omega(i)*dt;
       t(i+1) = t(i) + dt;
end

plot(t,theta,'r' );
xlabel('time (seconds) ');
ylabel('theta (radians)');
```

Solution 3

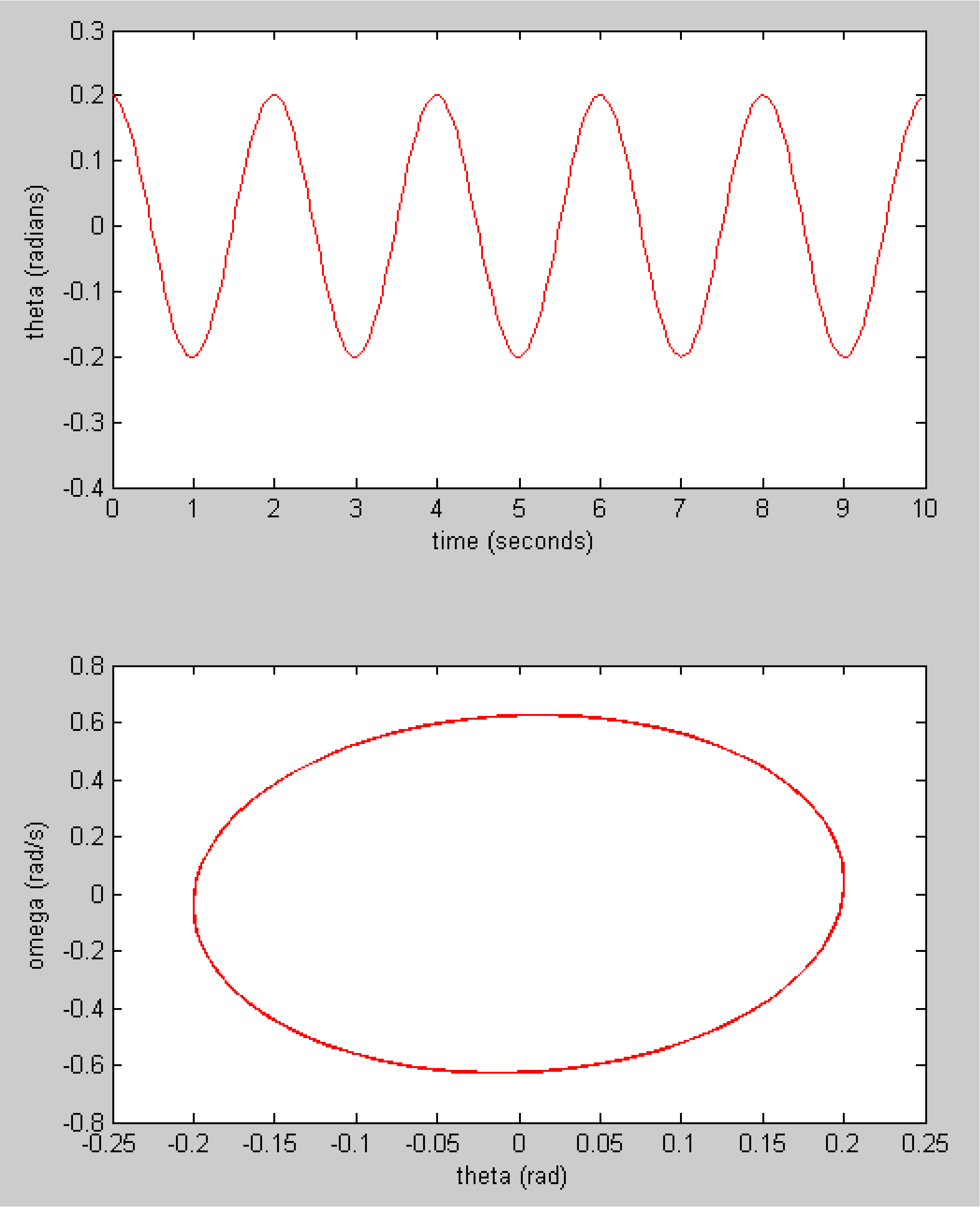

1.5
1
0.5
0
-0.5
-1
-1.5
0
1
2
3
4
5
6
7
8
9
10
theta (radians)
time (seconds)
6
4
2
0
-2
-4
-1.5
-1
-0.5
0
0.5
1
1.5
omega (rad/s)
theta (rad)

Solution 3

```
>> edit pendulum2.m
```

```
L = 1;      % length of the pendulum in meters
g = 9.8;    % acceleration due to gravity
n = 250;    % Discretize time into 250 intervals
dt = 0.04; % time step in seconds
omega = zeros(n,1);
theta = zeros(n,1);
t     = zeros(n,1);
theta(1) = 0.2;

for i = 1:n-1
   omega(i+1) = omega(i) - (g/L)*theta(i)*dt;
   theta(i+1) = theta(i) + omega(i+1)*dt;
       t(i+1) = t(i) + dt;
end

plot(t,theta,'r' );
xlabel('time (seconds) ');
ylabel('theta (radians)');
```

Solution 3


0.3
0.2
0.1
0
-0.1
-0.2
-0.3
-0.4
theta (radians)
0
1
2
3
4
5
6
7
8
9
10
time (seconds)
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
omega (rad/s)
-0.25
-0.2
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
0.2
0.25
theta (rad)

Example 4

Damped Pendulum:

$$\frac{d^2\theta}{dt^2} = -\frac{g}{L}\theta - q\frac{d\theta}{dt} \;\; ; \;\; \theta(0) = 0.2$$

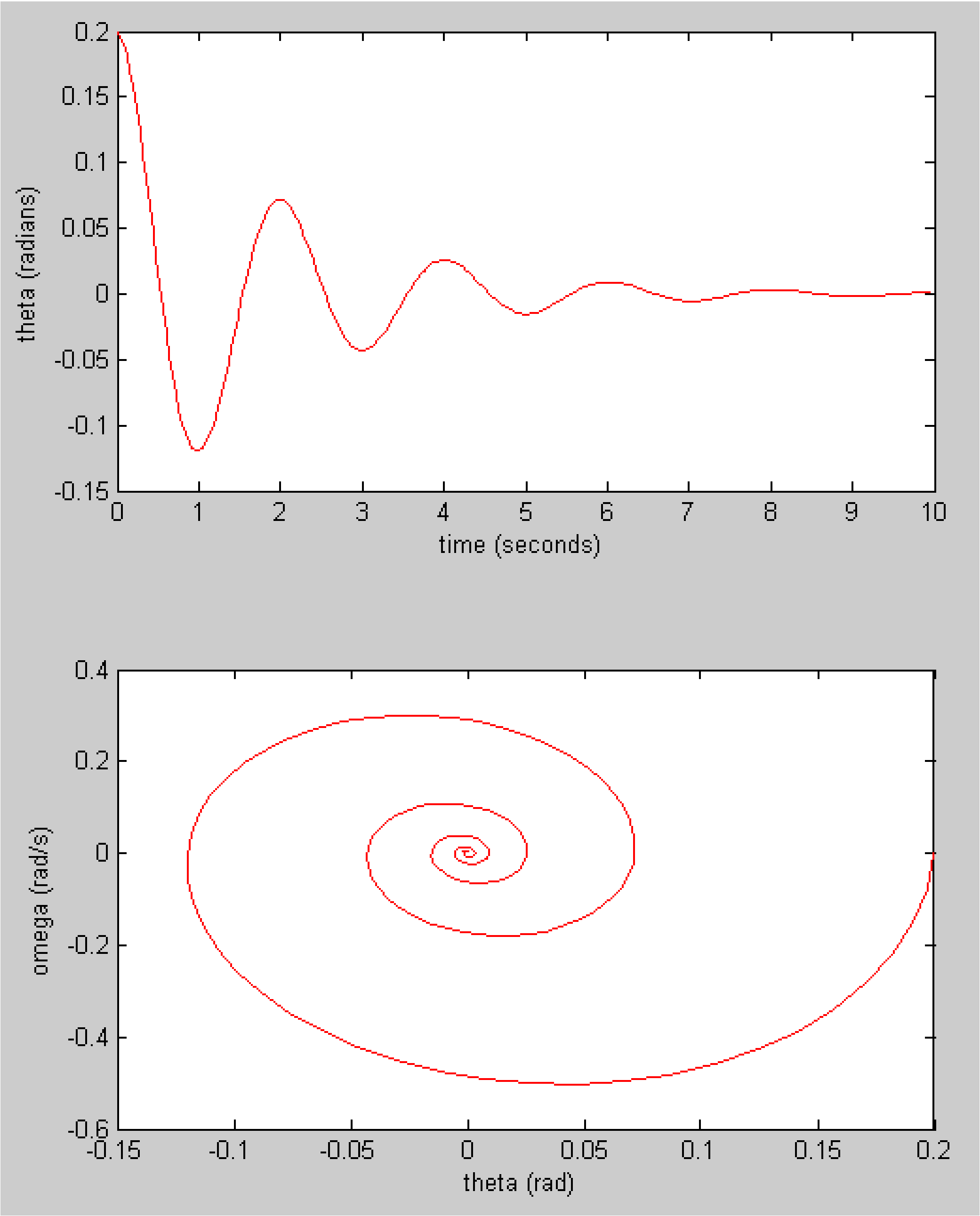
Find the numerical solution via Euler-Cromer method for dt = 0.04 s, L=1 m, n = 250 points and q=1.

Solution 4

```
>> edit pendulum3.m
```

```
L = 1;      % length of the pendulum in meters
g = 9.8;    % acceleration due to gravity
n = 250;    % Discretize time into 250 intervals
dt = 0.04; % time step in seconds
omega = zeros(n,1);
theta = zeros(n,1);
t     = zeros(n,1);
theta(1) = 0.2;
for i = 1:n-1
   omega(i+1) = omega(i) - (g/L)*theta(i)*dt - q*omega(i)*dt;
   theta(i+1) = theta(i) + omega(i+1)*dt;
       t(i+1) = t(i) + dt;
end
subplot(2,1,1);
    plot(t,theta,'r' );
    xlabel('time (seconds) ');
    ylabel('theta (radians)');
subplot(2,1,2);
    plot(theta,omega,'r' );
    xlabel('theta (rad) ');
    ylabel('omega (rad/s)');
```

Solution 4


theta (radians)
time (seconds)
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
0
1
2
3
4
5
6
7
8
9
10
omega (rad/s)
theta (rad)
0.4
0.2
0
-0.2
-0.4
-0.6
-0.15
-0.1
-0.05
0
0.05
0.1
0.15
0.2

Example 5

1D Schrödinger Equation for a particle of mass m is given by:

$$\frac{d^2\Psi(x)}{dx^2} = \frac{2m}{\hbar^2}(V(x) - E)\Psi(x); \quad \Psi(0) = 0, \Psi'(0) = 1$$

Let h-bar = m = 1, E = $\pi^2/8$ = 1.2337 and V(x) = 0.

Then:

$$\frac{d^2\Psi(x)}{dx^2} = -2E\Psi(x); \quad \Psi(0) = 0, \Psi'(0) = 1$$

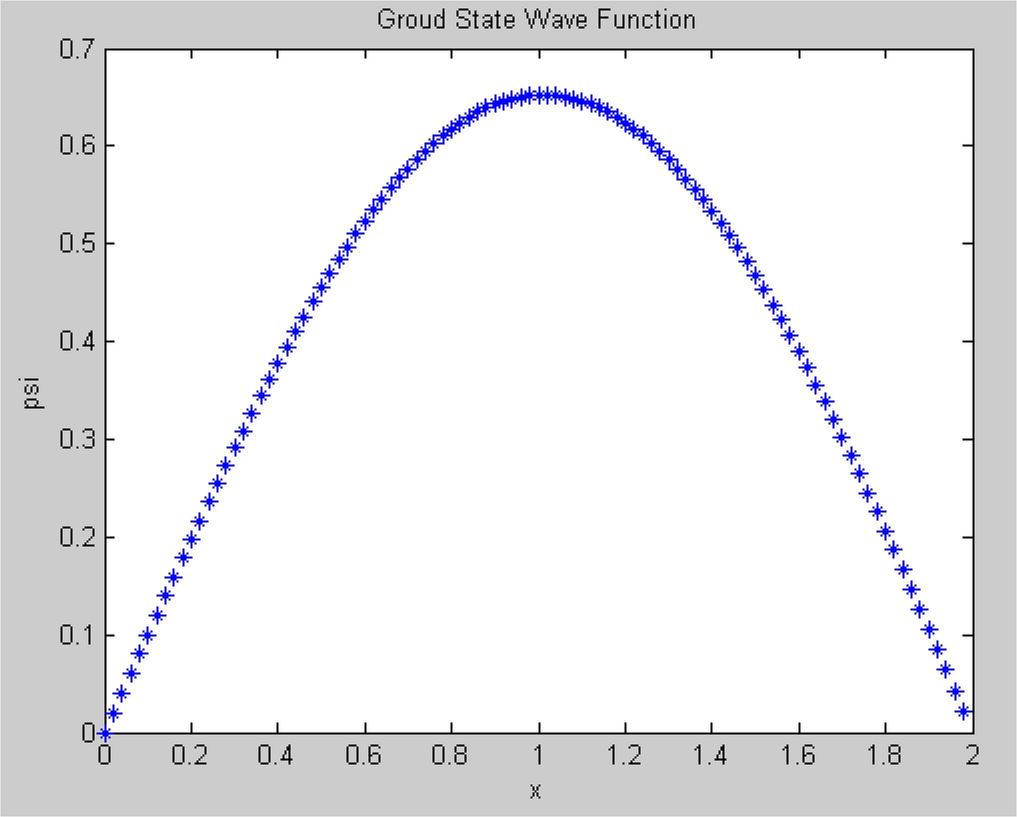
Find the numerical solution via Simple Euler method for the range 0<= x <= 2 and n = 100 points.

Solution 5

```
>> edit sch.m
```

```
function sch()
  x(1)= 0; u(1)= 1; y(1)= 0;

  n=100; E=pi^2/8;
  dx = 2/n;

  for i=1:n-1
      u(i+1) = u(i) - 2*E*y(i)*dx;
      y(i+1) = y(i) + u(i+1)*dx;
      x(i+1) = x(i) + dx;
      fprintf('%f  %f %f\n',x(i), u(i), y(i));
  end

  plot(x,y,'b*')
  xlabel('x')
  ylabel('psi')
  title('Groud State Wave Function')
end
```

Solution 5


Groud State Wave Function
psi
x
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
2

References:

[1]. Numerical Methods for Engineers, 6th Ed.
S.C. Chapra, Mc Graw Hill (2010)

[2]. http://www.mathworks.com/products/matlab

[3]. Numerical Methods in Engineering with MATLAB,
J. Kiusalaas, Cambridge University Press (2005)

[4]. Essential MATLAB for Engineers and Scientist, 3rd Ed
Hahn B., Valentine D.T. (2007)