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# -*- coding: utf-8 -*-  
"""
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Jonathan Ryding  
2nd yr Computational Physics, Project 2: Damped Harmonic Oscillator
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Program that uses four step-by step iterative methods to solve an unforced damped  
harmonic oscillator and compares with a solution calculated analytically.
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#Data is written to files then plotted from these files.
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Program shows the accuracy of the methods with varying step sizes.
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The best method, Verlet, is then used to solve the differential equation with  
driving forces for the analytically unsolved.
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Effects of driving forces (pulses and sinusoidals at varying frequencies) are  
viewed.
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@author: mclssjr6  
"""
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```
import numpy as np  
import matplotlib.pyplot as plt
```

```
#variables of the system, can be edited.
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```
k = 1.55 #spring constant of the oscillator [N / m]
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```
m = 5.81 #mass of ball
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```
b = 0 #damping coefficient
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```
omega0 = (k/m)**0.5
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```
omega = ((k / m) - pow((b/(2*m)),2) )**0.5 #oscillator angular frequency general  
for damped oscillations
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```
gamma = b/m #gamma constant
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```
b_crit = 2 *np.sqrt(k*m) #critical damping coefficient, defined where omega = 0
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#initial conditions of the oscillator, can be edited.
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x0 = 0 #initial displacement
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v0 = -1 #initial velocity
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h = 0.1 #step size used per iteration of each method
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#cannot choose h so small that round-off errors become significant
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time_tot = 100 #length of time desired to view oscillations
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```
def writeFile(file_name, time, X, V, E ):
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#Function that writes given data to a file.
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    file = open(file_name, "w")
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    print("Creating file: " + file_name + " for writing data into.")
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    for i in range(0, len(V)):
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        file.write("%f\t%f\t%f\t%f\n" %(time[i], X[i], V[i], E[i]) )
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    print("Writing completed, closing.")
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```
    file.close()
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```
    return(None)
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```
def readFile(file_name):
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#Function that reads data in from a file
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    opened = 0
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try:
#try to open the file, change a local variable if opens
    file = open(file_name, 'r')

    opened = 1

#file opened
except:

    print("Could not open file: " + file_name + " for reading in data.")

#file did not open, print a failure message

if opened is 1:

    file = np.loadtxt(file_name)

    X = np.array(file[:,1]) #position, in metres
    V = np.array(file[:,2]) #velocity, in metres per second
    E = np.array(file[:,3]) #total energy, in Joules

    return(X, V, E)

def time(time_total, h_step):
    N_points = int(time_total/h_step) #converts measuring time and step size into a
integer number of steps to do

#creating a time set that is universal across all functions
    t_time = np.zeros(N_points) #creating a zeros array with sufficient entries for
the given time desired

    for i in range(1, N_points):
        t_time[i] = i * h_step #progressing the time by steps to avoid small errors
functions such as np.linspace have for h steps that are not factors of the total
time, e.g. h = 0.3
#ensures time array is correct
    return(t_time, N_points)

def euler(file_name, x0, v0, h_step, N):
#Euler function
#Uses the Euler step-by-step iterative method to approximate numerically the damped
harmonic differential equation given initial conditions (as x0,v0)

    X, V, E = np.zeros(N), np.zeros(N), np.zeros(N-1)
    #X, V, E correspond to displacement, velocity and total energy respectively.
    #It is more memory efficient to create an array of size N than to append to an
empty array.

    X[0] = x0 #initial position and velocity are set into the arrays
    V[0] = v0

    for i in range(1, N): #calculate positions and velocities step-by-step until
the number of iterations, N, is reached.

        X[i] = X[i-1] + V[i-1] * h_step #Euler method:  $X_{n+1} = X_n + V_n * h$ 
#position local truncation error of order  $h^2$ , #taylor expansion
        V[i] = V[i-1] - ((b/m)*V[i-1] + (k /m)*X[i-1] ) * h_step # $V_{n+1} = V_n +$ 

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$a_n * h$  ,  $a_n$  is an acceleration

```
#velocity local truncation error of order  $h^2$ 
for i in range(0,N-1):
    E[i] =(m*V[i]**2/2 + k*X[i]**2/2)

#Remove last elements of position and velocity to data can be compared to
Verlet method (function below) where last velocity element cannot be calculated.
X = X[0:-1]
V = V[0:-1]

writeFile(file_name , t, X, V, E)
return(None)

def improvedEuler(file_name, x0, v0, h_step):
#Improved Euler method function
#Similar to the Euler method above, but the position, time-derivative of velocity,
an extra term from the Taylor expansion.

    X, V, E = np.zeros(N), np.zeros(N), np.zeros(N-1)
    #X, V, E correspond to displacement, velocity and total energy respectively.

    X[0] = x0 #initial position and velocity are set into the arrays
    V[0] = v0

    for i in range(1, N):

        X[i] = X[i-1] + V[i-1] * h_step - ((b/m)*V[i-1] + (k /m)*X[i-1] ) *
(h_step**2)/2 #extra term:  $a_n * h^2/2$  included
        #position local truncation error of order  $h^3$ , expected to be more accurate
        then previous Euler method.
        V[i] = V[i-1] - ((b/m)*V[i-1] + (k /m)*X[i-1] ) * h_step
        #velocity local truncation error of order  $h^2$ 

    for i in range(0,N-1):
        E[i] =(m*V[i]**2/2 + k*X[i]**2/2)

    X = X[0:-1]
    V = V[0:-1]

    writeFile(file_name , t, X, V, E)
    return(None)

def verlet(file_name, x0, v0, h_step, b_input, F):
#Verlet method function
#Uses Verlet method (position as the centred time- derivative) to calculate
solutions step-by-step.
#Requires an extra starting point from Euler method.
#Verlet was found to be the best method. Adjusted for inclusion of damping and a
varying input forces.

    X, V, E = np.zeros(N), np.zeros(N), np.zeros(N-1) #empty arrays are created for
position, velocity, energy

    X[0] = x0 #initial position and velocity are set into the arrays
    V[0] = v0

    X[1] = X[0] + h_step * V[0] #finding the first step using Euler method, then
```

continuing the iteration through with the Verlet method

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D = 2*m + b_input * h_step #calculating D,A,B Verlet coefficients.

A = 2*(2*m - k * (h_step**2) )/ D

B = (b_input*h_step - 2*m) / D

for i in range(2,N):

    X[i] = (A * X[i-1] + B * X[i-2] + 2*(h_step**2)*F[i-1]/D) # x2 acts as the
next step, x1 acts as current step, x0 acts as previous step.

    V[i-1] = (X[i] - X[i-2])/(2*h_step)

for i in range(0,N-1):
    E[i] =(m*V[i]**2/2 + k*X[i]**2/2)

X = X[0:-1]
V = V[0:-1]

writeFile(file_name , t, X, V, E)

return(None) #end of function

def eulerCromer(file_name, x0, v0, h_step):
#Euler- Cromer method function
#Uses the Euler-Cromer method to calculate solutions step-by-by step.
#The Euler-Cromer method is symplectic. Energy of the oscillator is preserved.
#Identical to the standard Euler method, except the position is calculated by using
the velocity at the next step.

    X, V, E = np.zeros(N), np.zeros(N), np.zeros(N-1) #empty arrays are created for
position, velocity, energy

    X[0] = x0 #initial position and velocity are set into the arrays
    V[0] = v0

    for i in range(1, N):
        #calculate solutions step-by-step until the time limit is reached
        V[i] = V[i-1] - ((b/m)*V[i-1] + (k /m)*X[i-1] )* h_step
        #V_n = V_n-1 + a_n-1 * h
        X[i] = X[i-1] + V[i] * h_step
        #X_n = X_n-1 + V_n

    for i in range(0,N-1):
        #calculate total at each point manually from kinetic energy + potential
energy
        E[i] =(m*V[i]**2/2 + k*X[i]**2/2)

    X = X[0:-1]
    V = V[0:-1]

    writeFile(file_name , t, X, V, E)

    return(None) #end of function

def analytical(file_name, x0, v0, t, h):
#analytically calculating given initial conditions. Works for light damping where
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omega is real.
#Useful website:
http://www.casaxps.com/help_manual/mathematics/Mechanics3_rev12.pdf

#Coefficients A, B calculated from initial conditions x0, v0.

A = x0/2 - 1j * (v0 + x0*gamma/2)/( 2 * omega)

B = x0 - A

X, V, E = np.zeros(N-1), np.zeros(N-1), np.zeros(N-1)
#It is more memory efficient to create an array of size N than to append to an
empty array.
#Length N-1 so number of data points is the same as found from the Verlet
method.

for i in range(0, N-1):

    X[i] = np.exp(-gamma*t[i]/2)*( A * np.exp(1j * omega* t[i]) + B * np.exp(-
1j*omega*t[i]) )
    #Calculating position at each point given the analytical solution X(t).
    V[i] = (1j*omega*(np.exp(-gamma*t[i]/2)) * (A * np.exp(1j * omega* t[i]) -
B * np.exp(-1j*omega*t[i]) ) - gamma*X[i]/2)
    #Calculating velocity at each point using the derivative of X(t) found
analytically.

    for i in range(0,N-1):
        #Calculating the total energy of the system at each point from kinetic and
potential energies summed.
        E[i] =(m*V[i]**2/2 + k*X[i]**2/2)

    writeFile(file_name , t, X, V, E)

    return(None)

def ComparisonOfMethods(Title, xAxis,yAxis, X, X1, X2, X3, X4, Y, Y1, Y2, Y3, Y4):
    #Graph plotter function
    #Plots data sets together

    if (X != "none"):
        plt.plot(X, Y, color = "g", label = "Analytical")
        plt.plot(X1, Y1, color = "b", label = "Euler")
        plt.plot(X2, Y2, color = "c", label = "Improved Euler")
        plt.plot(X3, Y3, color = "r", label = "Verlet")
        plt.plot(X4, Y4, color = "k", label = "Euler-Cromer")

        plt.legend(loc = "best")
        plt.title(Title)
        plt.xlabel(xAxis)
        plt.ylabel(yAxis)

        plt.show()

    #The methods can be compared by considering the total energy of the system. The
better methods will be closer to the real solutions calculated analytically.

def EnergyAreaDifference(Energy_method, Energy_analytical, time, h):
    #The ratio of the integrals of numerically calculated energies and the

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analytical with time can be used as a measure of how accurate a calculation method and step size are.

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Area_method = np.trapz(Energy_method, t[0:len(Energy_method)], h)
#integral = np.trapz(y(x), x , step_size)
#The integrals from the trapezium rule will be overestimates when the integrand
is increasing at a changing rate (concave up), and underestimates when the
integrand is concave down.
#This error is reduced by using smaller step sizes.
Area_analytical = np.trapz(Energy_analytical, t[0:len(Energy_analytical)], h)
Area_diff = Area_method - Area_analytical

return abs(Area_diff)

def energydifference(Energy_method, Energy_analytical):
    #The energy difference between solutions after some time for undamped
    simulations could be used to show how well the methods work.

    delta = np.zeros(len(Energy_method))

    for i in range(0, len(Energy_method)):
        delta[i] = ((Energy_method[i]) - Energy_analytical[i] /
Energy_analytical[i] )

    return delta

#main

#calling functions, then plotting position-time graphs for comparison
#no external force

t, N = time(time_tot, h)
Fnone = np.zeros(N)

analytical("fileanal.txt", x0, v0, t, h) #
Xanal, Vanal, Eanal = readFile("fileanal.txt")
t = t[0:-1]

euler("fileeuler.txt", x0, v0, h, N)
Xeuler, Veuler, Eeuler = readFile("fileeuler.txt")

improvedEuler("fileimprovedeuler.txt", x0, v0, h)
XimprovedEuler, VimprovedEuler, EimprovedEuler = readFile("fileimprovedeuler.txt")

verlet("fileverlet.txt", x0,v0, h, b, Fnone )
Xverlet, Vverlet, Everlet = readFile("fileverlet.txt")

eulerCromer("fileeulercromer.txt", x0, v0, h)
XeulCrom, VeulCrom, EeulCrom = readFile("fileeulercromer.txt")

ComparisonOfMethods("Displacement of four models against time", "Time,
s","Displacement, m", t, t, t, t, t, Xanal, Xeuler, XimprovedEuler, Xverlet,
XeulCrom)

ComparisonOfMethods("Phase space of four models", "Displacement, m","Velocity,
m/s", Xanal, Xeuler, XimprovedEuler, Xverlet, XeulCrom, Vanal, Veuler,
VimprovedEuler, Vverlet, VeulCrom)
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plt.yscale("log")
ComparisonOfMethods("Calculated energy of four models against time", "Time,
s", "Energy, J", t, t, t, t, t, Eanal, Eeuler, EimprovedEuler, Everlet, EeulCrom)
"""
#Efficiency with varying step size.
M = 3
H, effEuler, effimprovedEuler, effverlet, effeulCrom = np.zeros(M), np.zeros(M),
np.zeros(M), np.zeros(M) , np.zeros(M)

for i in range(0, (M-1)):
    H[i] = (h* 0.1**(i/4))
    t, N = time(time_tot, H[i])

    euler("fileeuler_%d.txt"%(i,), x0, v0, H[i], N)
    improvedEuler("fileeuler_%d.txt"%(i,), x0, v0, H[i])
    verlet("fileeuler_%d.txt"%(i,), x0,v0, H[i], b, Fnone)
    eulerCromer("fileeuler_%d.txt"%(i,), x0, v0, H[i])

    Xeuler, Veuler, Eeuler = readFile("fileeuler_%d.txt"%(i,))
    XimprovedEuler, VimprovedEuler, EimprovedEuler = readFile("fileimprovedeuler_
%d.txt"%(i,))
    Xverlet, Vverlet, Everlet = readFile("fileverlet_%d.txt"%(i,))
    XeulCrom, VeulCrom, EeulCrom = readFile("fileeulercromer_%d.txt"%(i,))

    Deuler =energydifference(Eeuler, Eanal)
    DimprovedEuler =energydifference(EimprovedEuler, Eanal)
    Dverlet =energydifference(Everlet, Eanal)
    DeulCrom =energydifference(EeulCrom, Eanal)

    effEuler[i] = max(Deuler)
    effimprovedEuler[i] = max(DimprovedEuler)
    effverlet[i] = max(Dverlet)
    effeulCrom[i] = max(DeulCrom)

plt.scatter(H, effEuler, color = "b", label = "Euler")
plt.scatter(H, effimprovedEuler, color = "c", label = "Improved Euler")
plt.scatter(H, effverlet, color = "r", label = "Verlet")
plt.scatter(H, effeulCrom, color = "k", label = "Euler-Cromer")

plt.title("Efficiency of models against step size")
plt.xlabel("Step size")
plt.ylabel("Efficiency")
plt.legend(loc = "best")
#energy accuracy
#calculations are more accurate if they are close to the analytical
"""
h = 0.01
t, N = time(time_tot, h)

analytical("fileanal.txt", x0, v0, t, h) #
Xanal, Vanal, Eanal = readFile("fileanal.txt")

t = t[0:-1]

#Using Verlet method for b = b_crit/2 (1), b_crit (2) and 2*b_crit (3)
Fnone = np.zeros(N)

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#Plotting verlet for different damping coefficients

verlet("verletdamped1.txt", x0, v0, h, b_crit/2, Fnone)
Xverlet1, Vverlet1, Everlet1 = readFile("verletdamped1.txt")

verlet("verletdamped2.txt", x0,v0, h, b_crit, Fnone)
Xverlet2, Vverlet2, Everlet2 = readFile("verletdamped2.txt")
#

verlet("verletdamped3.txt", x0, v0, h, 2*b_crit, Fnone)
Xverlet3, Vverlet3, Everlet3 = readFile("verletdamped3.txt")

plt.plot(t, Xverlet1, label = "Verlet")

plt.title("Verlet damping, with b_crit/2")
plt.xlabel("Time, s")
plt.ylabel("Position, m")
plt.show()
#More than one complete oscillation.

plt.plot( t, Xverlet2, label = "Verlet")
plt.title("Verlet critical damping")
plt.xlabel("Time, s")
plt.ylabel("Position, m")
plt.show()

#One half complete oscillation, with the minimum disturbance time.

plt.plot( t, Xverlet3, label = "Verlet")
plt.title("Verlet damping, with 2*b_crit")
plt.xlabel("Time, s")
plt.ylabel("Position, m")
plt.show()
#One half complete oscillation, but the disturbance time is longer than at the
critical damping.
"""

#sudden application of external force for damping coefficient b

Fext = np.zeros(N)
for i in range((int(N/4)), int(3*N/4)):
    Fext[i] = 70

verlet("verletforced1.txt", x0, v0, h, b, Fext)
Xverlet4, Vverlet4, Everlet4 = readFile("verletforced1.txt")

plt.plot(t, Xverlet4)

plt.xlabel("t, s")
plt.ylabel("Position, m")
plt.show()

Fext = np.zeros(N)

for i in range((int(N/4)), int(N-1)):

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    Fext[i] = np.sin(omega * t[i]) #resonant frequency

verlet("verletforced1.txt", x0, v0, h, b, Fext)
Xverlet5, Vverlet5, Everlet5 = readFile("verletforced2.txt")

plt.plot(t, Xverlet5)

plt.xlabel("t, s")
plt.ylabel("Position, m")
plt.show()

for i in range((int(N/4)), int(N-1)):
    Fext[i] = np.sin(2* omega * t[i]) #double the resonant frequency

Xverlet4, Vverlet4, Everlet4 = verlet(x0,v0, b, Fext)

plt.plot(t, Xverlet4)
plt.xlabel("t, s")
plt.ylabel("Position, m")
plt.show()

for i in range((int(N/4)), int(N-1)):
    Fext[i] = np.sin(t[i]) #some rother frequency

plt.plot(t, Xverlet4)

plt.xlabel("t, s")
plt.ylabel("Position, m")
plt.show()

"""

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