Computation in Classical Mechanics

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Scientific advances create the need to become computationally adept to tackling problems of increasing complexity. The use of computers in attaining solutions to many of science's difficult problems is inevitable. Therefore, educators face the challenge to infuse the undergraduate curriculum with computational approaches that will enhance students' abilities and prepare them to meet the world's newer generation of problems. Computational physics courses are becoming part of the undergraduate physics landscape and learned skills need to be honed and practiced. A reasonable ground to do so is the standard traditional upper level physics courses. I have thus developed a classical mechanics $textbook¹$ that employs computational techniques. The idea is to make use of numerical approaches to enhance understanding and, in several cases, allow the exploration and incorporation of the "what if environment" that is possible through computer algorithms. The textbook uses Matlab because of its simplicity, popularity, and the swiftness with which students become proficient in it. The example code, in the form of Matlab scripts, is provided not to detract students from learning the underlying physics. Students are expected to be able to modify the code as needed. Efforts are under way to build OSP2 Java programs that will perform the same tasks as the scripts. Selected examples that employ computational methods will be presented. ¹ To be published, Jones and Bartlett Publishers.

² Open Source Physics: http://www.opensourcephysics.org/.

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Why we need computational physics? We can go beyond solvable problems. We can get more insight. We can explore situations beyond classroom examples.

Start with the iterative Euler method.

Chapter 1 Highlights

Why we need computational physics? We can go beyond solvable problems. We can get more insight. We can explore situations beyond classroom examples.

If we know the acceleration of an object,

$$
\int dv = \int a \, dt
$$

If the acceleration is constant, an object's velocity is

$$
v(t) = v_0 + at \quad \Rightarrow \qquad \int dx = \int v(t)dt \quad \Rightarrow \qquad x(t) = x_0 + v_0 t + \frac{1}{2}at^2
$$

However, if the acceleration is not constant, say a mass at the end of a spring,

$$
\oint \sqrt{k} \sqrt{m} \sqrt{m} \sqrt{k} \sqrt{k} = -kx(t) \qquad a(t) = -kx(t)/m = \frac{d^2x}{dt^2} = \frac{dv}{dt}
$$

The analytic solution is done in a later chapter. Let's look at a numerical solution. MATLAB code is provided. Students are encouraged to run it and explore it.

•The Euler Method to solve a 2nd order DE: convert it to two 2nd order DE's

$$
\frac{dx}{dt} = v(t, x) \quad \text{and} \quad \frac{dv}{dt} = a(t, v) \quad \text{So that we do,}
$$
\n
$$
v_{i+1} = v_i + a_i \Delta t, \quad x_{i+1} = x_i + v_{i+1} \Delta t \quad \text{to be solved on } [t_0, t_f] \quad \text{with}
$$
\n
$$
t_{i+1} = t_i + \Delta t, \quad a_i = -k x_i / m. \quad \text{For N steps} \quad \Delta t = (t_f - t_0) / N
$$
\nGiven initial conditions:

\n
$$
x_0, \quad v_0
$$

First example, by calculator (reproduced by a general force MATLAB code): let $k = 1000N/m$, $m = 5kg$, $x_0 = 0.1m$, $v_0 = 0.0m/s$ on time interval [0,1*s*]

for $N = 10$ so that $\Delta t = 0.1$

•Create a table of the calculations

•Can create a plot of this rough calculation


```
%ho1.m
%Calculation of position, velocity, and acceleration for a harmonic
%oscillator versus time. The equations of motion are used for small time intervals
clear;
%NPTS=100;TMAX=1.0;%example Maximum number of points and maximum time
TTL=input(' Enter the title name TTL:','s');%string input
NPTS=input(' Enter the number calculation steps desired NPTS: ');
TMAX=input(' Enter the run time TMAX: ');
NT=NPTS/10;%to print only every NT steps
%K=1000;M=5.0;C=0.0;E=0.0;W=0.0;x0=0.1;v0=0.0;% example Parameters
K=input(' Enter the Spring contant K: ');
M=input(' Enter the bob mass M: ');
C=input(' Enter the damping coefficient C: ');
E=input(' Enter the magnitude of the driving force E: ');
W=input(' Enter the driving force frequency W: ');
x0=input(' Enter the initial position x0: ');% Initial Conditions
v0=input(' Enter the initial velocity v0: ');% Initial Conditions
t0=0.0;% start at time t=0dt=TMAX/NPTS;%time step size
fprintf(' Time step used dt=TMAX/NPTS=%7.4f\n',dt);%the time step being used
F=-K*x0-C*v0+E*sin(W*t0); % initial force
a0=F/M;% initial acceleration
fprintf(' t x - y = a \ln');% output column labels
v(1)=v0;x(1)=x0;a(1)=a0;t(1)=t0;fprintf('%7.4f %7.4f %7.4f %7.4f\n',t(1),x(1),y(1),a(1));%print initial values
for i=1:NPTSv(i+1)=v(i)+a(i)*dt; % new velocity
  x(i+1)=x(i)+v(i+1)*dt; %new position
  t(i+1)=t(i)+dt; % new time
  F=-K*x(i+1)-C*v(i+1)+E*sin(W*t(i+1)); %new force
  a(i+1)=F/M; % new acceleration
% print only every NT steps
  if(mod(i,NT)=0)fprintf('%7.4f %7.4f %7.4f %7.4f\n',t(i+1),x(i+1),y(i+1),a(i+1));
  end;
end;
```
ho1.m continued on next page

ho1.m continued from previous page

 $subplot(3,1,1)$ $plot(t, x, 'k-)$; $ylabel'(x(t) (m)$, FontSize', 14); h=legend('position vs time'); set(h,'FontSize',14); title(TTL,'FontSize',14); $subplot(3,1,2)$ $plot(t, v, 'b-)$; ylabel('v(t) (m/s)','FontSize',14); h=legend('velocity vs time'); set(h,'FontSize',14) $subplot(3,1,3)$ $plot(t,a,'r-');$ ylabel('a(t) (m/s^2) ','FontSize',14); xlabel('time (sec)','FontSize',14); h=legend('acceleration vs time'); set(h,'FontSize',14)

•We also need to be able to visualize analytical solutions – so use small MATLAB scripts provided or modify available ones

•**Harmonic Motion example: Interacting Spring-Mass System (Computation)** Interaction massspring system a)with walls, and b) without walls d^2 2 2 $m_2 \frac{d^2 x_2}{dt^2} = -k_2 x_2 - k_0 (x_2 - x_1)$

$$
m_1 \frac{d^2 x_1}{dt^2} = -k_1 x_1 - k_0 (x_1 - x_2)
$$
 and $m_2 \frac{d^2 x_2}{dt^2} = -k_2 x_2 - k_0 (x_2 - x_1)$

 $k_1 = k_2 = 0$ 2 $\Lambda_1(\nu) = \lambda_{cm}(\nu)$ λ_{cm0} $1 \frac{1}{2}$ $f(t) = x_{cm}(t) - x_{cm0} - \frac{m_2}{\sqrt{m_2}} x_r(t)$ *m* $x_1(t) = x_{cm}(t) - x_{cm0} - \frac{m_2}{t} - x_r(t)$ $= x_{cm}(t) - x_{cm0} - \frac{m_2}{m_1 + m_2} x_r(t) \Bigg[x_2(t) = x_{cm}(t) - x_{cm0} + \frac{m_1}{m_1 + m_2}$ $2(v) - \lambda_{cm}(v)$ λ_{cm0} $1 \cdot m_2$ $f(t) = x_{cm}(t) - x_{cm0} + \frac{m_1}{r} x_r(t)$ *m* $x_2(t) = x_{cm}(t) - x_{cm0} + \frac{m_1}{t} - x_r(t)$ $m_1 + m$ $= x_{cm}(t) - x_{cm0} +$ + •Case 1: No Walls - Single Mode $k_1 = k_2 = 0$ The analytic solution is:

$$
x_r = A \sin \omega t + B \cos \omega t
$$
, $\omega A = v_{r0} = v_{20} - v_{10}$, $B = x_{r0} = x_{20} - x_{10}$

$$
x_{cm}(t) - x_{cm0} = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} = v_{cm}t \qquad v_{cm} = \frac{m_1 v_1 + m_2 v_2}{m_1 + m_2} = \frac{m_1 v_{10} + m_2 v_{20}}{m_1 + m_2}
$$

•Can create a plot of this calculation inter spr1.html

•Case2: Full System - Bimodal $m_1 = m_2 = m$, $k_1 = k_2 = k \neq k_0$

Write the equations in the matrix form $m \ddot{x} = -k x - k_0 M x$

where
$$
m \equiv \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix}
$$
 $x \equiv \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ $k \equiv \begin{pmatrix} k & 0 \\ 0 & k \end{pmatrix}$ $M \equiv \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$

Solve using eigenvalue-eigenvector method, get two modes $x_1(t) = x_{10} \cos \overline{\omega} t \cos \omega_m t + x_{20} \sin \overline{\omega} t \sin \omega_m t$ $x_2(t) = x_{10} \sin \overline{\omega} t \sin \omega_m t + x_{20} \cos \overline{\omega} t \cos \omega_m t$ Average frequency Modulation frequency $\overline{\omega} = (\omega_1 + \omega_2)/2$ Modulation
frequency $\omega_m = (\omega_2 - \omega_1)/2$

•Can create a plot of this calculation inter_spr2.html

• **Three Dimensional Motion** of a **charged Particle in an Electromagnetic Field (Computation)** - This follows the two dimensional analytic solutions of the charge in Electric, magnetic, and joint E& B fields

We have

$$
\vec{F} = q\vec{v} \times \vec{B} + q\vec{E} = m\vec{a}
$$
 or

$$
\frac{d^2x}{dt^2} = q(v_yB_z - v_zB_y + E_x)/m, \quad \frac{d^2y}{dt^2} = q(v_zB_x - v_xB_z + E_y)/m, \quad \frac{d^2z}{dt^2} = q(v_xB_y - v_yB_x + E_z)/m
$$

In MATLAB write these as

$$
x \to r(1)
$$
, $\dot{x} \to r(2)$; $y \to r(3)$, $\dot{y} \to r(4)$; $z \to r(5)$, $\dot{z} \to r(6)$

Obtain six 1st order equations given by

$$
\frac{dr(1)}{dt} = r(2), \quad \frac{dr(2)}{dt} = q[r(4)B(3) - r(6)B(2) + E(1)]/m
$$

$$
\frac{dr(3)}{dt} = r(4), \quad \frac{dr(4)}{dt} = q[r(6)B(1) - r(2)B(3) + E(2)]/m
$$

$$
dr(5) = dr(6)
$$

$$
\frac{dr(5)}{dt} = r(6), \quad \frac{dr(6)}{dt} = q[r(2)B(2) - r(4)B(1) + E(3)]/m
$$

where we have the field arrays E_y, E_z) = $E(1, 2, 3),$ $B = (B_x, B_y, B_z) = B(1, 2, 3)$ Field values example: $E = [0.5 \times 10^{-8}, 1 \times 10^{-9}, -3 \times 10^{-9}]$, $B = [1 \times 10^{-8}, -1 \times 10^{-9}, 5.13 \times 10^{-8}]$

• see cycloid3d.html

A charged particle moving in the presence of a three dimensional electromagnetic field

Systems of Coordinates - Foucault pendulum (computation)

S-frame (Earth's center) acceleration: $\vec{a} = -g \hat{k}' + \vec{T}/m = \ddot{\vec{r}}' + 2\vec{\omega} \times \dot{\vec{r}}' + \vec{\omega} \times (\vec{\omega} \times \vec{r}')$ Look at x-y plane motion, and ignore $\vec{\omega} \times (\vec{\omega} \times \vec{r}')$, but keep the Coriolis term, and

 -0.6 -0.8

-1 L
-1

 -0.8

 -0.6

 -0.4

 -0.2

 $\overline{0}$

 0.2

 0.4

 0.6

 0.8

See Foucault.html

Gravitation: Binary Mass System Simulation

Center of mass of a binary mass system

$$
\vec{r}_2 = \vec{r}_{cm} + \frac{m_1}{m} \vec{r}
$$

Can write an equation for each mass

$$
m_1 \frac{d^2 \vec{r}_1}{dt^2} = -\frac{Gm_1 m_2 \vec{r}_1}{r_{12}^3}, \quad m_2 \frac{d^2 \vec{r}_2}{dt^2} = -\frac{Gm_1 m_2 \vec{r}_2}{r_{21}^3} \qquad \vec{r} = \vec{r}_2 = -\vec{r}_1 = -\vec{r}_1 = -\vec{r}_1 = -\vec{r}_1
$$

 $m_1\tilde{r}/m$

 \vec{r}_1

т.

But can also use Center of Mass - Relative Coordinate Method

Binary System, CM-Rel. Coord. Method: tau = 6.988 tau_n, m₁ = 3 m_s, m₂ = 2 m_s 4

Using astronomical units

see and binary1.html binary1.avi

Binary system simulation using analytic formulas

Rutherford Scattering (simulation)

Motion of Rigid Bodies – Symmetric Top (simulation)

Using ة لآل $\bar{\psi} \propto$ $v''' = 2$ Eulerian Spinning symmetric top with its Cm symmetry axis (), which is its angles spin axis as well as its principal γ", L.· ϕ , θ , ψ axis of symmetry, at angle from mg the fixed axis $\vec{\tau} = \left(\frac{d\vec{L}}{dt}\right) = \left(\frac{d\vec{L}}{dt}\right) + \vec{\omega}'' \times \vec{L} = mg\ell$ $\vec{\tau} = \left(\frac{d\vec{L}}{dt}\right)_{fixed} = \left(\frac{d\vec{L}}{dt}\right)_{rot} + \vec{\omega}'' \times \vec{L} = mg \ell \sin \theta \hat{i}''$ $x^m = 1$ $\left(\frac{d\bar{L}}{d\bar{L}}\right)$ = $\left(\frac{d\bar{L}}{d\bar{L}}\right)$ + $\bar{\omega}'' \times \bar{L}$ = $mg \ell \sin \theta \hat{i}$ $\sin \theta \hat{i}$ $x' = x'', L_x$ *fixed* $\langle u \rangle$ *rot* $\vec{L} = I \dot{\theta} \hat{i}'' + I \dot{\phi} \sin \theta \hat{j}'' + I_s \omega_s \hat{k}''$, $\vec{\omega}'' = \dot{\theta} \hat{i}'' + \dot{\phi} \sin \theta \hat{j}'' + \dot{\phi} \cos \theta \hat{k}''$ $I_3(\dot{\varphi}\cos\theta + \dot{\psi}) \equiv I_s\omega_s$ or $mg \ell \sin \theta = I \ddot{\theta} + I_s \omega_s \dot{\phi} \sin \theta - I \dot{\phi}^2 \cos \theta \sin \theta$ solve numerically for $0 = I \frac{d}{dt} (\dot{\phi} \sin \theta) - I_s \omega_s \dot{\theta} + I \dot{\theta} \dot{\phi} \cos \theta$ $= I \frac{d}{dt} (\dot{\phi} \sin \theta) - I_s \omega_s \dot{\theta} + I \dot{\theta} \dot{\phi} \cos \theta$ $\phi(t), \theta(t), \psi(t)$ *dt* $0 = I_s \dot{\omega}_s$ (a) (b) Top Euler Angles: φ₀=0, θ₀=0.95, ψ₀=0 rad dφ/dt_n=0, dθ/dt_n=0, ω_n=2.5 rad/s Top V_{ett}(θ): φ_n=0, θ_n=0.95, ψ_n=0 rad, dφ/dt_n=0, dθ/dt_n=0, ω_s=2.5 rad/s 0.67 =1, 1.5 kgm², M=1kg <u>호</u>05 05 $\overline{\theta}_1$, $\overline{\theta}_2$ = 0.952, 1.08 rad, E'=0.568 J 0.565 g=9.8 m/s², a=0.1 m
I, I_=1, 1.5 kgm², M=1kg 0 $\tilde{\mathbf{u}}$ = 0.56

මේ
>ී0.555

 0.55

 0.545

 0.54
 0.94

 0.96

 0.98

 $z'' = z''' = 3, L.$

z, L,

 $\frac{1}{2}$ ക 0.9 -0.5 2.6 30 $\overline{20}$ $rac{1}{2}$ ² \Rightarrow (c)

Top motion: φ_n=0, θ_n=0.95, ψ_n=0 rad, dφ/dt_n=0, dθ/dt_n=0, ∞_s=2.5 rad/s

spinning fixed point symmetric top a) Numerical solution, b) Plot of the energy and the effective potential, and c) a snapshot of the simulated motion of the top's total angular momentum as well as the body angular momentum vs time

 1.02

1.04

1.06

See top.html and top.avi

LAGRANGIAN DYNAMICS – Double Pendulum (simulation)

Double Pendulum

Coordinates

 $x_1 = L_1 \sin \theta_1$ $x_2 = x_1 + L_2 \sin \theta_2$ $y_1 = L_1 \cos \theta_1$ $y_2 = y_1 + L_2 \cos \theta_2$

kinetic, potential energies

$$
T = \frac{1}{2}m_1(\dot{x}_1^2 + \dot{y}_1^2) + \frac{1}{2}m_2(\dot{x}_2^2 + \dot{y}_2^2), \quad V = m_1gL_2 + m_1gh_1 + m_2g(h_1 + h_2)
$$

\nLagrangian
\n
$$
L = T - V = \frac{1}{2}m_1L_1^2\dot{\theta}_1^2 + \frac{1}{2}m_2\left[L_1^2\dot{\theta}_1^2 + L_2^2\dot{\theta}_2^2 + 2L_1L_2\dot{\theta}_1\dot{\theta}_2\cos(\theta_1 - \theta_2)\right] - m_1gL_2 - (m_1 + m_2)gL_1(1 - \cos\theta_1) - m_2gL_2(1 - \cos\theta_2).
$$

\nequations
\n• solve
\n
$$
\begin{aligned}\n(m_1 + m_2)L_1\ddot{\theta}_1 + m_2L_2\ddot{\theta}_2\cos(\theta_1 - \theta_2) &= -m_2L_2\dot{\theta}_2^2\sin(\theta_1 - \theta_2) - (m_1 + m_2)g\sin\theta_1 \\
m_2L_2\ddot{\theta}_2 + m_2L_1\ddot{\theta}_1\cos(\theta_1 - \theta_2) &= m_2L_1\dot{\theta}_1^2\sin(\theta_1 - \theta_2) - m_2g\sin\theta_2\n\end{aligned}
$$

See doublep.html and doublep.avi

The double pendulum a) Eulerian angles plotted versus time (upper figure) and versus each other (lower figure) b) simulation of the pendulum for the initial conditions shown.

LAGRANGIAN DYNAMICS – Principle of Least Action (simulation)

Hamilton's principle: the motion followed by a mechanical system as it moves from a starting point to a final point within a given time will be the motion that provides an extremum for the time integral of the Lagrangian.

Example – case of a particle in free fall, we have the Lagrangian and the action:

$$
L = T - V = \frac{1}{2} m v_y^2 - mgy
$$
\n
$$
S = \int_{t_0}^{t_f} L dt = \int_{t_0}^{t_f} \left(\frac{1}{2} m v^2 - mgy \right) dt
$$

Numerically, make the approximation:

$$
= \int_{t_0}^{t_f} L dt \approx \Delta t \sum_{k=1}^{N-1} L_k
$$
 with $L_k = L(t_k) \approx \frac{1}{2} m \left(\frac{y_{k+1} - y_k}{\Delta t} \right)^2 - m g y_k$
and the initial guess $\longrightarrow y_k = y_0 + \frac{(y_f - y_0)}{(t_f - t_0)} (t_k - t_0)$

Modify the guess randomly, accept steps that lead to s decrease in $dS = S_{n,N-1} - S_{n-1,N-1}$

until dS is small. Compare numerical results against the exact solution

$$
y = y_0 + v_0 t - \frac{1}{2}gt^2
$$

 Ω

Simulation of Hamilton's least action principle for the case of the motion of a single particle free falling near Earth's surface, in one dimension

0

 $S =$

See least_action.html and least action.avi

Other Highlights

•Harmonic oscillator (undamped, damped, and forced)

•Projectile Motion (analytic and numerical)

•The pendulum (small, and large angles)

•Central Forces -Planetary Motion (analytic, numerical, and simulations) and comparison with data

•Eulerian Angle Frame Rotation (visualization)

•More on Rutherford Scattering --Comparison with the 1913 Geiger Marsden Data for Silver and Gold

Conclusion

•A junior level mechanics textbook has been developed that incorporated computational physics: "Intermediate Classical Mechanics with MATLAB applications."

•The text makes use of the valuable traditional analytic approach in pedagogy. It further incorporates computational techniques to help students visualize, explore, and gain insight to problems beyond idealized situations.

•Some programming background is expected and most physics/engineering majors have had programming experience by their junior year.

•The emphasis is placed on understanding. The analytic approach is supported and complemented by the computational approach.

•Java applications analogue to the MATLAB scripts are available (under development) see below. They use the Open Source Physics (OSP) library of W. Christian and co-workers. <http://www.westga.edu/~jhasbun/osp/osp.htm> <http://www.opensourcephysics.org/>

•Comments are welcome. Please contact J. E. Hasbun jhasbun@westga.edu

OPEN SOURCE PHYSICS (OSP) JAVA APPLICATIONS

ho1app

inter_spr1App

inter_spr2App

cycloid3dApp

foucaultApp

binary1App

rutherApp

topApp

least_actionApp

