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Numerical Methods in Physics
Solution of Lagrange's and Hamilton's equations of motion
for a symmetric top

PURPOSE: To compare the Lagrangian and Hamiltonian formalisms.
To compare numerical solutions obtained with the Runge-Kutta and Bulirsch-Stoer method, respectively.
To use physical principles to control the accuracy of a numerical solution.

LITERATURE:

M. Galassi *et al.*, GNU Scientific Library Reference Manual, 2nd ed. (Network Theory, Bristol, 2006), <http://www.gnu.org/software/gsl/>
W. H. Press *et al.*, Numerical Recipes in C, 2nd ed. (Cambridge University Press, Cambridge, 1992), chap. 16, <http://www.nrbook.com/a/bookcpdf.php>

¹Based on work by Sune Pettersson, Anna Jonsson, and Tord Oscarsson.

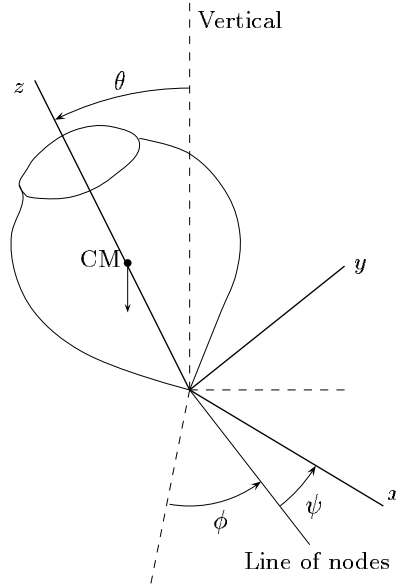


Figure 1: Relation between the Euler angles describing the orientation of the top and a fixed Cartesian coordinate system.

1 Introduction

In this exercise we study the motion of a symmetric top. The kinetic energy K for the top can be written as

$$K = \frac{1}{2}I_1(\omega_1^2 + \omega_2^2) + \frac{1}{2}I_3\omega_3^2 \quad (1)$$

where I_3 is the moment of inertia relative to the symmetry axis of the top, and I_1 is the moment of inertia about an axis through the tip, directed perpendicular to the symmetry axis. The angular velocity of the rotation about the symmetry axis is denoted by ω_3 while ω_1 and ω_2 are the angular velocities around two axes going through the tip and perpendicular to both the symmetry axis and to each other.

Figure 1 introduces the Euler angles, whose relation to the angular velocities are given by

$$\omega_1 = \dot{\phi} \sin \theta \sin \psi + \dot{\theta} \cos \psi \quad (2)$$

$$\omega_2 = \dot{\phi} \sin \theta \cos \psi - \dot{\theta} \sin \psi \quad (3)$$

$$\omega_3 = \dot{\phi} \cos \theta + \dot{\psi}. \quad (4)$$

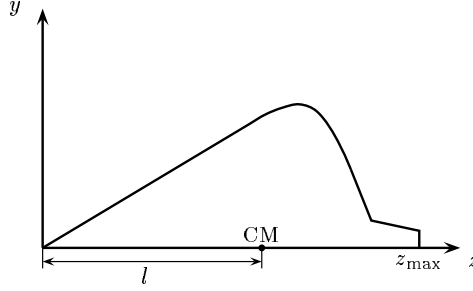


Figure 2: $y(z)$ defines the shape of the symmetric top.

We can write the kinetic energy in terms of the Euler angles as

$$K = \frac{I_1}{2} (\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta) + \frac{I_3}{2} (\dot{\psi} + \dot{\phi} \cos \theta)^2. \quad (5)$$

The potential energy, V , is obtained by summing over all particles in the top

$$V = - \sum_i m_i \mathbf{r}_i \cdot \mathbf{g}, \quad (6)$$

where \mathbf{g} is the gravitational acceleration. By denoting the position of the center of mass of the top by \mathbf{R} we get

$$V = -M\mathbf{R} \cdot \mathbf{g} \quad (7)$$

where M is the mass of the top. With the origin placed at the tip we finally obtain

$$V = Mgl \cos \theta. \quad (8)$$

2 The moment of inertia

An arbitrary symmetric top can be described by a function $y(z)$, which gives the perpendicular distance from a point on the symmetry axis to the surface of the top (see figure 2). The density can vary along the symmetry axis, and is denoted by $\rho(z)$. The total mass of the top is

$$M = \int_0^{z_{\max}} \rho(z) \pi y^2(z) dz. \quad (9)$$

Due to symmetry, the center of mass has to lie on the symmetry axis and we get

$$Ml = \int_0^{z_{\max}} \rho(z) \pi y^2(z) z dz, \quad (10)$$

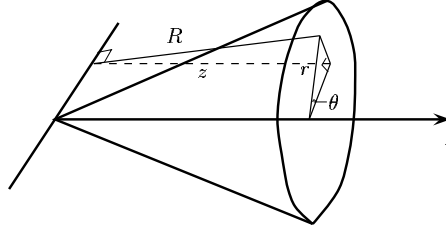


Figure 3: Definition of the variables r and R used when determining the moment of inertia about an axis through the tip of the top and perpendicular to the symmetry axis.

such that l can be recovered from the ratio of the two integrals.

The moment of inertia about the symmetry axis is given by:

$$\begin{aligned}
 I_3 &= \int \rho(\mathbf{r}) r^2 dV \\
 &= \int_0^{z_{\max}} dz \int_0^{2\pi} d\theta \int_0^{y(z)} dr \rho(z) r^2 r \\
 &= \frac{\pi}{2} \int_0^{z_{\max}} \rho(z) [y(z)]^4 dz,
 \end{aligned} \tag{11}$$

where we have introduced cylindrical coordinates to evaluate integral.

The moment of inertia about an axis through the tip of the top and perpendicular to the symmetry axis is given by

$$\begin{aligned}
 I_1 &= \int \rho(z) R^2 r dr d\theta dz \\
 &= \int \rho(z) (z^2 + r^2 \sin^2 \theta) r dr d\theta dz \\
 &= \pi \int_0^{z_{\max}} \rho(z) [y(z)]^2 z^2 dz + \frac{\pi}{4} \int_0^{z_{\max}} \rho(z) [y(z)]^4 dz
 \end{aligned} \tag{12}$$

where r and R are defined in figure 3.

Exercise 1

Write a program that calculates M , l , I_1 and I_3 when functions returning $y(z)$ and $\rho(z)$ are given. The integrals can be calculated using adaptive integration with singularities, `gsl_integration_qags`. Check your program by

calculating the variables above for a well known object (*e.g.*, a homogeneous cylinder or a homogeneous cone). Reasonable values for the tolerances are `expabs = 1e-8` and `exprel = 1e-12`.

In the directory `~fnm/top/` there are several object files which define symmetrical tops, `topn.o`. Each defines two functions, `double top_y(double z)` and `double top_rho(double z)`, which return $y(z)$ and $\rho(z)$, respectively. The units of z and y is cm, ρ is given in g/cm^3 , and all tops extend from $z = 0$ to 5 cm.

These functions are declared in `top.h` and are interchangeable between object files, *i.e.*, the same program can be used for any of the tops just by linking to the appropriate object file. Determine M , l , I_1 and I_3 for one of the tops.

Bonus exercise

Reverse engineer the functions in the `topn.o` files to recover the analytical formulas for the different $y(z)$ and $\rho(z)$. Using these formulas, calculate the exact values of M and compare to the result of the numerical integration. How does it vary with `expabs` and `exprel`, and how good is the error estimate `abserr`? Compare also the algorithms QAG, QAGS, and QAGP. In the latter case, the singular points correspond to discontinuities in the derivative.

3 Lagrange's equations of motion

Our first attempt to describe the motion of the top is to solve Lagrange's equations of motion numerically. We start by constructing the Lagrangian,

$$\begin{aligned} L &= K - V \\ &= \frac{I_1}{2} (\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta) + \frac{I_3}{2} (\dot{\psi} + \dot{\phi} \cos \theta)^2 - Mgl \cos \theta \end{aligned} \quad (13)$$

The general form of Lagrange's equations of motion is

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{q}_j} \right) - \frac{\partial L}{\partial q_j} = 0 \quad (14)$$

where q_j denotes the generalized coordinates. In our Lagrangian we have three coordinates and thereby obtain three equations of motion:

$q_j = \theta$:

$$\frac{d}{dt} (I_1 \dot{\theta}) = \left[I_1 \dot{\phi}^2 \sin \theta \cos \theta + I_3 (\dot{\psi} + \dot{\phi} \cos \theta) \dot{\phi} (-\sin \theta) + Mgl \sin \theta \right] \quad (15)$$

or

$$I_1 \left(\ddot{\theta} - \dot{\phi}^2 \sin \theta \cos \theta \right) + I_3 \left(\dot{\psi} + \dot{\phi} \cos \theta \right) \dot{\phi} (-\sin \theta) - Mgl \sin \theta = 0 \quad (16)$$

$q_j = \phi$:

$$\frac{d}{dt} \left[I_1 \dot{\phi} \sin^2 \theta + I_3 \left(\dot{\psi} + \dot{\phi} \cos \theta \right) \cos \theta \right] - 0 = 0 \quad (17)$$

or

$$I_1 \dot{\phi} \sin^2 \theta + I_3 \left(\dot{\psi} + \dot{\phi} \cos \theta \right) \cos \theta = \text{constant} \quad (18)$$

$q_j = \psi$:

$$\frac{d}{dt} \left[I_3 \left(\dot{\psi} + \dot{\phi} \cos \theta \right) \right] = 0 \quad (19)$$

or

$$I_3 \left(\dot{\psi} + \dot{\phi} \cos \theta \right) = \text{constant} \quad (20)$$

One way to attack this system of second order ordinary differential equations is to rewrite them so that the second derivatives only depend on the first derivatives and the functions themselves. After some algebra the Lagrangian equations of motion can be written on the form

$$\ddot{\phi} = \frac{I_3}{I_1} \left[\frac{\dot{\phi} \dot{\theta} \cos \theta}{\sin \theta} + \frac{\dot{\psi} \dot{\theta}}{\sin \theta} \right] - 2\dot{\theta} \dot{\phi} \cot \theta \quad (21)$$

$$\ddot{\psi} = \dot{\phi} \dot{\theta} \sin \theta + 2\dot{\theta} \dot{\phi} \frac{\cos^2 \theta}{\sin \theta} - \frac{I_3}{I_1} \left[\frac{\dot{\phi} \dot{\theta} \cos^2 \theta}{\sin \theta} + \dot{\psi} \dot{\theta} \cot \theta \right] \quad (22)$$

$$\ddot{\theta} = \frac{Mgl}{I_1} \sin \theta + \dot{\phi}^2 \sin \theta \cos \theta - \frac{I_3}{I_1} \left(\dot{\psi} + \dot{\phi} \cos \theta \right) \dot{\phi} \sin \theta. \quad (23)$$

Exercise 2

Rewrite the equations above as a system of six first order ordinary differential equations, and write a program for solving them numerically. For the integration of the ODEs, use the Runge-Kutta-Fehlberg method, implemented in the function `gsl_odeiv_step_rkf45`, with constant time steps (*i.e.*, use `gsl_odeiv_step_apply`).

Use the program from exercise 1 as a subroutine so that you easily can choose which top to solve the equations of motion for.

Let the angle between the top and the vertical line be $\theta = 20^\circ$ and it's rotational velocity $\dot{\psi} = 10$ revolutions/s. The other Euler angles and angular velocities are put to zero at $t = 0$ s. Calculate how the top moves during the next 4 seconds.

Show how the Euler angles and the corresponding angular velocities are varying with time. Describe in your own words how the top is moving during these 4 seconds.

Several quantities should be constant in time. Energy has to be conserved as the forces originate from a conservative potential. Check that the energy is conserved between $t = 0$ and 4 s. Two other constants of motion are defined by eqs. (18) and (20). Check the conservation of these two constants too. If any of the constants varies with time the step size may be too large.

To further check of the reliability of the solution, run the program backwards from $t = 4$ s. That is, change the sign of the time step and take as start values the end values you obtained for $t = 4$ s. If the step size is small enough you will regain the initial values at $t = 0$ s.

When you look carefully at the results you might see that some of the tops will crash into the table given the initial conditions above. If you like, and have the time, you can add a test that checks if the top is touching the table. You may also try to alter the initial conditions so that this does not happen.

4 Hamilton's equations of motion

Since the generalized coordinates do not depend explicitly on time and the forces originate from a conservative potential we can write

$$\begin{aligned} H &= K + V \\ &= \frac{I_1}{2} (\dot{\theta}^2 + \dot{\phi}^2 \sin^2 \theta) + \frac{I_3}{2} (\dot{\psi} + \dot{\phi} \cos \theta)^2 + Mgl \cos \theta. \end{aligned} \quad (24)$$

The conjugated momenta, defined by

$$p_i = \frac{\partial L(q_j, \dot{q}_j, t)}{\partial \dot{q}_i}, \quad (25)$$

then become

$$p_\psi = \frac{\partial L}{\partial \dot{\psi}} = I_3 (\dot{\psi} + \dot{\phi} \cos \theta), \quad (26)$$

$$p_\phi = \frac{\partial L}{\partial \dot{\phi}} = (I_1 \sin^2 \theta + I_3 \cos^2 \theta) \dot{\phi} + I_3 \dot{\psi} \cos \theta, \quad (27)$$

$$p_\theta = \frac{\partial L}{\partial \dot{\theta}} = I_1 \dot{\theta}. \quad (28)$$

After some algebraic work, we can rewrite our Hamiltonian as a function of q_j and p_j ,

$$H = \frac{p_\theta^2}{2I_1} + \frac{(p_\phi - p_\psi \cos \theta)^2}{2I_1 \sin^2 \theta} + \frac{p_\psi^2}{2I_3} + Mgl \cos \theta. \quad (29)$$

Hamilton's equations of motion can generally be written as

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad (30)$$

$$-\dot{p}_i = \frac{\partial H}{\partial q_i}. \quad (31)$$

In this context an advantage with Hamilton's equations compared to Lagrange's equations is that Hamilton's equations are already written as a system of first order ordinary differential equations.

Exercise 3

Derive Hamilton's equations of motion for the top. If you do this correctly you will get four equations of motion to solve. The other two equations of motion defines two constants of motion, which are identical to those we found with Lagrange's equations of motion.

Write a program for solving Hamilton's equations of motion using the Bulirsch-Stoer method. Note that the algorithm `gsl_odeiv_step_bsimp` requires a Jacobian. Use the same initial conditions as in exercise 2. Compute the constants of motion to verify that they are conserved by the numerical scheme. Compare the Hamiltonian solution to that obtained in exercise 2 using the Lagrange/Runge-Kutta method.

5 Presentation of results

Present your results in a **brief** report. Write as little text as possible, just present what is required by the instructions:

- Instructions for how to compile and run the programs written for exercise 1, 2, and 3.
- A table over the results obtained in exercise 1.
- The six first order equations used in exercise 2.

- A program listing of the function implementing the Lagrangian ODEs.
- Diagrams showing how ϕ , ψ , and θ varies with time in exercise 2.
- Diagrams from exercise 2 showing the conservaton of energy and eqs. (18) and (20).
- A diagram showing what happens when the solution in exercise 2 is reversed in time.
- Hamilton's equations used in exercise 3.
- The Jacobian for Hamilton's equations.
- Diagrams showing how ϕ , ψ , and θ varies with time in exercise 3.