MATHEMATICAL MODELING FOR PHYSICAL SCIENCES

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ABSTRACT. Abstract goes here :)

CONTENTS

1. GUIDE

This section provides with guidelines to approach the mathematical modeling of physical phenomena.

1.1. **Problem background.** A mathematical model of a physical phenomenon begins with the *problem background*, a description or introduction to the object. It should contain

- a *description* of the essential features of the physical process and
- an identification of the *objectives*, the key questions requiring answers.

Answering what, who, where, how and why questions guides to write down the description. Additionally, including graphical illustrations aids not only in the description, but in the definition of physical quantities and the establishment of hypotheses, as well.

1.2. **Problem formulation.** The *problem formulation* aims to:

- identify key physical processes;
- interpret these processes mathematically;
- establish a mathematical model – governing equations and suitable initial and boundary conditions;
- state clearly the assumptions.

The formulation must be based on sound physical principles, experimental facts or laws expressed in mathematical terms. As a guide, then, define the physical framework (geometry, kinematics, dynamics, thermal transfer and so on), state a dimensional set and then define the physical quantities, constants, parameters, coefficients and provide their dimensions in the chosen set.

A more formal approach is to begin with educated guessing, followed by dimensional analysis, order of magnitude analysis [1], analysis of extreme cases, simplifications and ends with a restricted model. The end result may be less accurate to fit experimental data, but less complex and thus more understandable. If fitting is not satisfactory, one can relax simplifications, one at a time, until a desired, or required, agreement is found.

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[1]Order of magnitude analysis is preceded by dimensional analysis, since *only* the comparison of *dimensionless* quantities is meaningful!

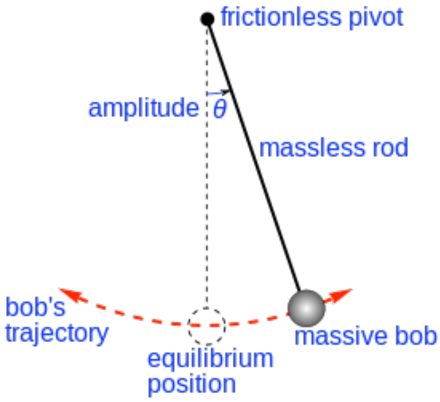

FIGURE 1. Schema of a simple gravitational pendulum

1.3. **Analysis.** Once the physical and mathematical models and their assumptions have been proposed, one regularly faces a set of equations, probably differential equations together with initial and boundary conditions. The next step is then to analyze the set by

- non-dimensionalize the equations, included initial and boundary conditions;
- making analogies with other related problems or phenomena, as the case of mass, energy and momentum transport and
- relying on analytic and numeric methods, obtaining solutions (results).

In the case of obtaining analytic solutions to differential equations, it is necessary to verify that they satisfy the differential equations object to the initial and boundary conditions.

As a final step, uncertainty analysis should be performed, to obtained ranges of validity, instead of punctual solutions.

1.4. **Results.** The final step of modeling physical phenomena is to present results, give conclusions and discussion them. Specifically, one should

- interpret results with respect to the original physical process and objectives;
- verify assumptions by confronting the results with reference values or experimental data and
- identify the solution limitations and possible extensions.

2. Description

[In this section, we set the description of a physical phenomenon: the motion of a gravitational pendulum. We focus on answer the questions: what is a pendulum? what is a gravitational pendulum? How the pendulum is set into motion? What keeps the pendulum moving? What forces act on the pendulum that damp its motion?]

A pendulum is a mechanical system consisting of a bob hanging by a rod attached, in turn, to a pivot, see fig. 1. A gravitational pendulum is a pendulum object only to gravitational interactions.

There are basically three ways of setting a gravitational pendulum into motion:

(1) by moving the bob from its equilibrium position to an initial angle, θ_0, at time $t = 0$;
(2) by applying a force that imprints an angular velocity to the bob, $\dot{\theta}_0$, at time $t = 0$;
(3) or by both at the same time $t = 0$.

Once the pendulum is swinging, an interplay between kinetic energy and gravitational potential energy keeps the system in motion. Kinetic energy initiates motion by the initial displacement or initial forces that perturbed the system from its equilibrium position, while the gravitational potential tries to restore the bob to its equilibrium position. This

Quantity	Symbol	Dimension
pendulum amplitude	θ	1
initial amplitude	θ_0	1
time	t	T
free fall acceleration	g	L/T^2
rod length	l_{rod}	L
rod mass	m_{rod}	M
torque at pivot	τ	ML^2/T
pivot friction coefficient	α	1
bob mass	m_{bob}	M
bob density	ρ_{bob}	M/L^3
bob diameter	d_{bob}	L
fluid density	ρ_{fl}	ML^3
fluid dynamic viscosity	μ	M/LT

Table 1. Physical quantities involved in the motion of a gravitational pendulum

interplay will continue indefinitely, unless damping forces, eventually, stop the pendulum from moving. Friction on the pivot or drag – if the pendulum is partially or totally submerged in a viscous fluid – are examples of damping forces.

3. Objective

To seek for a mathematical relation, perhaps in a closed form, to predict the pendulum amplitude variation with time; *i.e.*, deduce a function of the form $\theta[t]$.

4. Physical processes

A swinging gravitational pendulum is an instance of a dynamics process, since a description of motion, based on its causes, is the final aim.

There are two main cases to consider when studying the motion of a gravitational pendulum: undamped motion, where no frictional forces and no drag are taken into account, and damped motion, where frictional forces or drag are considered. In both cases, however, the interplay between kinetic energy and gravitational potential must be regarded, since it drives motion.

To uncover the relationships between the different physical quantities that affect the pendulum motion, we follow a plan: propose the quantities that may affect motion; then, join them as dimensionless quantities and, finally, use physical considerations and order of magnitude analysis to restrain the physical model, decreasing thus complexity. The last step will pave the path to a precise mathematical model.

4.1. **Dimensional and order of magnitude analyses.** We consider first the most complex case: a gravitational pendulum hanging by a massive rod joint to a dry and clean pivot. The pendulum swings through a viscous fluid.

Since the problem belongs to dynamics, we choose the dimensional set $\{\mathsf{L}, \mathsf{M}, \mathsf{T}\}$, with a cardinality of three. Next, let us list the possible physical quantities that may influence the pendulum motion together with their symbols and dimensions [2], see table 1.

A first approach may be to model the pendulum amplitude by a function f of the form

$$\theta = f[\theta_0, t, g, l_{\mathrm{rod}}, m_{\mathrm{rod}}, \tau, \alpha, m_{\mathrm{bob}}, \rho_{\mathrm{bob}}, d_{\mathrm{bob}}, \rho_{\mathrm{fl}}, \mu]\ .$$

This complex relationship can be organized by means of dimensional analysis.

To begin with, since ρ_{bob}, m_{bob} and d_{bob} are related, we can keep two of the three quantities. We keep diameter and density. With this reduction, there are 12 physical quantities and 3 independent dimensions. Thus, according to the Pi-theorem, the number

[2] The equation for the friction at the pivot is $\tau = \alpha m g r$, where α is the friction coefficient, m the mass supported by the pivot and r the radius of the axis or rod supporting the pivot.

of dimensionless quantities that can be formed is $12-3=9$. These dimensionless quantities may be chosen as

$$\Pi_1 = \theta\,,\ \Pi_2 = \theta_0\,,\ \Pi_3 = t\sqrt{\frac{g}{l}}\,,$$
$$\Pi_4 = \alpha\,,\ \Pi_5 = \frac{m_{\text{rod}}}{m_{\text{bob}}}\,,\ \Pi_6 = \frac{(m_{\text{bob}} + m_{\text{rod}})\, g l_{\text{rod}}}{\tau}\,,$$
$$\Pi_7 = \frac{d}{l}\,,\ \Pi_8 = \frac{\rho_{\text{fl}}}{\rho_{\text{bob}}}\,,\ \Pi_9 = \frac{\rho_{\text{fl}} d\sqrt{lg}}{\mu}\,.$$

See that Π_1 contains the quantity being sought, θ, that Π_2 the quantity that originates motion, θ_0, and Π_3 the (independent) quantity against which we confront motion, t. Now, again using the Pi-theorem, the mathematical function we seek, ψ, is of the *form*:

$$\theta = \psi\left[\theta, \theta_0, t\sqrt{\frac{g}{l}}, \alpha, \frac{m_{\text{rod}}}{m_{\text{bob}}}, \frac{(m_{\text{bob}} + m_{\text{rod}})\, g l_{\text{rod}}}{\tau}, \frac{d}{l}, \frac{\rho_{\text{fl}}}{\rho_{\text{bob}}}, \frac{\rho_{\text{fl}} d\sqrt{lg}}{\mu}\right]\,. \tag{4.1}$$

To reduce the complexity of the mathematical model, we can restrain the physical model by working on the pendulum, by doing order of magnitude analysis and by making assumptions.

First, friction at the pivot can be reduced by properly lubricating the joint between the pivot and the rod. With this, the frictional torque term disappears – a frictionless pivot. To support this assumption, let us bring some numbers. A dry and clean joint of steel pivot and steel rod has a friction coefficient of 0.80, while when the joint is lubricated the coefficient decreases to 0.16.

Next, the rod may be build of a strong material; strong enough to support the bob without elongating. This will allow the construction of a very thin rod. This implies, in turn, that the ratio of masses can be neglected – a massless, inflexible rod.

We use now order of magnitude analysis to further restrain the model. Consider that the rod length is much greater than the bob length. This is possible since we are building the pendulum with a very strong rod. Some numbers: if the bob diameter is, say, 5 cm and the rod length 1 m, then the ratio $d/l = 0.05$.

Our pendulum may be swinging through air. Then, the bob density will be greater than the air density. For instance, if the bob is made of steel and swings through air at 15 °C and at sea level, then

$$\rho_{\text{air}}/\rho_{\text{steel}} = 1.225\,\text{kg/m}^3/7750\,\text{kg/m}^3 \sim 0.158 \times 10^{-4}\,,$$

which can be ignored [3].

Air can be considered as an inviscid fluid. An inviscid fluid is a fluid with no viscosity, then drag will not be crucial. To back up this assumption, plug some typical values into Π_9:

$$\frac{\rho_{\text{air}} d_{\text{bob}}\sqrt{lg}}{\mu} = \frac{1.225 \times 0.05\sqrt{1.00 \times 9.80665}}{1.983 \times 10^{-5}} \sim 9672\,,$$

where values in SI units were used. It can be seen that inertial forces, $\rho_{\text{air}} d_{\text{bob}}\sqrt{lg}$, are much larger than viscous forces, μ, meaning that the latter may be safely discarded.

As a side note, considering the pivot to be frictionless and no drag present – undamped pendulum case – implies that mechanical energy is conserved. Then, the system may be analyzed using Lagrange formulation of mechanics, instead of Newton formulation.

Finally, after having restrained the physical model, we seek for a mathematical function of the form

$$\theta = \psi\left[\theta_0, t\sqrt{\frac{g}{l}}\right]\,. \tag{4.2}$$

Neither dimensional analysis nor order of magnitude analysis can help to find the functional form of ψ. It must be found by a more refined theoretical analysis or by experimentation. However, our assumptions, based on sensible assumptions, have reduced the complex, physical model by passing from 13 dimensional quantities to 3 dimensionless quantities.

[3] However, if the steel bob swings through oil with $\rho_{\text{oil}} = 850\,\text{kg/m}^3$, then $\rho_{\text{oil}}/\rho_{\text{steel}} = 850\,\text{kg/m}^3/7750\,\text{kg/m}^3 \sim 0.110$, which may be important for some applications.

At the end of the day, however, only confrontation of the model with experimental data will provide the accuracy of the reductions we have done.

Some final words. Equation (4.2) may seem, at first sight, a very restricted model. However, it is a practical one: the pendulum of a longcase clock. Such a clock consists of a heavy bob hanging by a light, inflexible and practically massless rod. The pendulum swings inside a case full of air.

4.2. **Mathematical interpretation.** For the gravitational pendulum, we begun seeking a mathematical relationship of the form presented in eq. (4.1). Then, after sensible physical considerations were made, we ended with a restricted model of the form eq. (4.2).

The physical considerations we made translate mathematically into

- A frictionless pivot implies no torque. Thus, $\Pi_4 = \Pi_6 = 0$.
- A massive bob hanging of a massless and inflexible rod implies that $\Pi_5 = 0$.
- A bob diameter much smaller than rod length results in $\Pi_7 = 0$.
- A bob made of steel swinging through air, air being less dense than steel, gives $\Pi_8 = 0$.
- Air considered as inviscid, implies no viscosity, thus no drag. Therefore, $\Pi_9 = 0$.

Finally, for the sake of mathematical purposes, we can combine all the previous assumptions by defining a *simple gravitational pendulum*:

> a simple gravitational pendulum is a pendulum composed of a massive bob of mass m hanging by a massless, frictionless and inflexible rod of length l attached to a frictionless pivot. Under the influence of gravitational interactions, the pendulum swings through an inviscid fluid of negligible density.

4.3. **Mathematical model.** In this section, we deduce the equation of motion for a simple gravitational pendulum by means of Lagrange formulation mechanics. Writing down the Lagrangian is possible due to the fact that the system is assumed to be undamped – conservative; *i.e.*, neither friction nor drag are considered. Additionally, we assume that the pendulum is set into motion by displacing the bob an initial angle θ_0 with no further forces, $\dot{\theta}_0 = 0$.

Consider a simple gravitational pendulum composed of a bob of mass m and a rod of length l. Let θ be the amplitude of the pendulum for any time t, let the initial angle be θ_0 and the initial velocity be $\dot{\theta}_0 = 0$ and, finally, let g be the free fall acceleration. Then, find the equation of motion for the pendulum.

Using θ as the generalized position and $\dot{\theta}$ as the generalized velocity, write down the Lagrangian for the system:

$$e_{\text{lag}} = \frac{1}{2} m l^2 \dot{\theta}^2 - mgl\left(1 - \cos[\theta]\right) .$$

Find next the generalized momentum and its temporal change

$$\partial_{\dot{\theta}} e_{\text{lag}} = m l^2 \dot{\theta} \implies \mathrm{d}_t \partial_{\dot{\theta}} e_{\text{lag}} = m l^2 \ddot{\theta} .$$

Calculate the generalized force:

$$\partial_{\theta} e_{\text{lag}} = -mgl \sin[\theta] .$$

Replace the generalized force and the temporal change of the generalized momentum in the Euler-Lagrange equation to find:

$$\Box_{\theta\dot{\theta}} e_{\text{lag}} = \partial_{\theta} e_{\text{lag}} - \mathrm{d}_t \partial_{\dot{\theta}} e_{\text{lag}} = -mgl \sin[\theta] - m l^2 \ddot{\theta} = 0 \implies m l^2 \ddot{\theta} + mgl \sin[\theta] = 0 .$$

Since $ml > 0$, divide the last equation through ml^2 to have

$$\ddot{\theta} + \frac{g}{l} \sin[\theta] = 0 ,$$

object to the initial conditions $\theta[0] = \theta_0$ and $\dot{\theta}[0] = \dot{\theta}_0 = 0$. Finally, rewrite the last equation as

$$\begin{cases} \dfrac{\mathrm{d}^2\theta}{\mathrm{d}t^2}[t] + \dfrac{g}{l}\sin[\theta[t]] = 0\,, \\ \theta[0] = \theta_0\,, \\ \dfrac{\mathrm{d}\theta}{\mathrm{d}t}[0] = \dot{\theta}_0 = 0\,. \end{cases} \tag{4.3}$$

4.4. **Assumptions.** The equation of motion for the pendulum was found using the assumptions made in section 4.1 and summarized in section 4.2.

5. Analysis

In this section, we solve the mathematical model proposed in section 4.3; *i.e.*, we solve eq. (4.3).

5.1. **Non-dimensional analysis.** First, non-dimensionalize the model. The independent quantity is t, the dependent quantity θ and the parameters are θ_0, l and g. Since θ is already dimensionless, we only have to non-dimensionalize t. We can do this by using Π_3 obtained in section 4.1. Thus,

$$\bar{t} = \Pi_3 = t\sqrt{\frac{g}{l}} \implies t = \bar{t}\sqrt{\frac{l}{g}}$$

and

$$\mathrm{d}t = \mathrm{d}\bar{t}\sqrt{\frac{l}{g}} \implies \mathrm{d}t^2 = \mathrm{d}\bar{t}^2\,\frac{l}{g}\,.$$

Replacing both equations in eq. (4.3) and dividing the result through g/l, we have

$$\begin{cases} \ddot{\theta} + \sin[\theta] = 0\,, \\ \theta[0] = \theta_0\,, \\ \dot{\theta}[0] = 0\,, \end{cases} \tag{5.1}$$

where the derivatives are to be taken with respect to $\bar{t}$. Note that the eq. (5.1) is dimensionless and parameter free.

5.2. **Analytic solution.** Equation (5.1) is a non-linear, second-order ordinary differential equation. We can linearize it by restraining θ to values less than 1 rad (*aka*, small-angle approximation). With this, $\sin[\theta] \sim \theta$ and therefore

$$\begin{cases} \ddot{\theta} + \theta = 0\,, \\ \theta[0] = \theta_0\,, \\ \dot{\theta}[0] = 0\,, \end{cases}$$

where the error due to the approximation is of order θ^3. The solution to this equation is

$$\theta\left[\bar{t}\right] = \theta_0 \cos\left[\bar{t}\right]\,,$$

or, returning to the dimensional quantity t,

$$\theta[t] = \theta_0 \cos\left[t\sqrt{\frac{g}{l}}\right]\,, \tag{5.2}$$

which gives the desired result.

6. Results

Equation (5.2) is the final mathematical model to the description of motion of a simple gravitational pendulum. Although restrained both physically and mathematically with respect to the original problem – a non-simple pendulum, the solution does provide a closed form function to predict the pendulum amplitude variation with time.

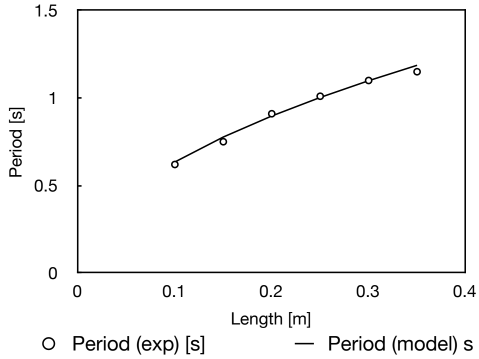

FIGURE 2. Model values for the simple gravitational pendulum and experimental data gathered from a real gravitational pendulum

6.1. **Discussion.** The motion described by eq. (5.2) is *simple harmonic motion*, where θ_0 is the semi-amplitude of the oscillation – the maximum angle between the rod of the pendulum and the vertical. The period of the motion, τ, the time for a complete oscillation – outward and return, is then

$$\tau_0 = 2\pi\sqrt{\frac{g}{l}}\,,$$

which is known as *Christiaan Huygens's law for the period*. Note that under the small-angle approximation, the period is independent of the amplitude θ_0; this is the property of *isochronism* that Galileo discovered.

6.2. **Experimental data and reference values.** Experimental data was not specifically gathered for writing the present document. However, some reference values were found in the internet [source!]. Such values together with the model predictions of eq. (5.2) are presented in fig. 2.

Using fig. 2, one finds that the *coefficient of determination*, R^2, between model figures and experimental data is 0.9876, while the relative error 2.03 %. Both figures show agreement between model and experiment, thus eq. (5.2) is taken to correctly represent real pendula.

Nevertheless, if more accuracy is required or less agreement is found when applying eq. (5.2) to a real pendulum, then the model can be extended by relaxing the assumptions made in section 4.4. For instance, if the pendulum swings through a viscous fluid, such as a liquid, then the dimensionless quantities Π_8 and Π_9 should be included. Or, if there is little care in lubricating the pivot, then Π_4, Π_5 and Π_6 should be further studied.