Physible: Interactive Physics Collection
MA198 Proposal Rough Draft

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November 6th 2015

Abstract

Physible conglomerates four smaller, physics-related programs into one package. Each subprogram features a 3-D simulation of some physical system, which are interactive to varying degrees. Ranging from simple kinematics to quantum mechanics, Physible will demonstrate visually the mathematics behind simulations of real-world physical systems, thereby making the physics visible.

1 Introduction and Background

Physible will combine four sub-programs into one, user-browsable interface. The user may not only view each program at their leisure, but will be able to interact with them by actually entering values to view how they reflect differences in the outcome. These four sub-programs vary in conceptual complexity and are samples of the following disciplines: kinematics, chaos theory, quantum mechanics, and thermal and statistical physics. Because of the number of sub-programs, which could easily be programs on their own if delved into deeply enough, they will be more surface-level explorations and examples, but could be later added onto for another project.

1.1 Kinematics

The kinematics project is the most simple: it displays the path of motion of some thrown object under the effects of gravity. The relevant equations are derived from the assumption of constant gravitational force and the definitions of acceleration and velocity:

$$\vec{a}_y = \frac{d\vec{v}_y}{dt} = -g\hat{y}$$

$$\vec{v}_y = \frac{d\vec{y}}{dt} = \int_0^t \vec{a}_y dt = (v_{y_0} - gt)\hat{y}$$

$$\vec{y} = \int_0^t \vec{v}_y dt = (y_0 + v_{y_0} t - \frac{1}{2} g t^2)\hat{y}$$

and so given an initial velocity and position, we know the position of the object for all times t. Because there are no forces in the $\hat{x}$ or $\hat{z}$ directions, their accelerations are zero and thus their velocities constant (until the object hits the ground).

1.2 Chaos Theory

The chaos project features the paradigm of chaos: a double-pendulum system. This system is most easily described through the approach of Lagrangian mechanics[1]. With this, we can describe the position of each pendulum as a function of its angle with respect to its pivot, and using the Euler-Lagrange equations, we can solve for their motion. Figure 1[2] displays how the coordinates are measured.

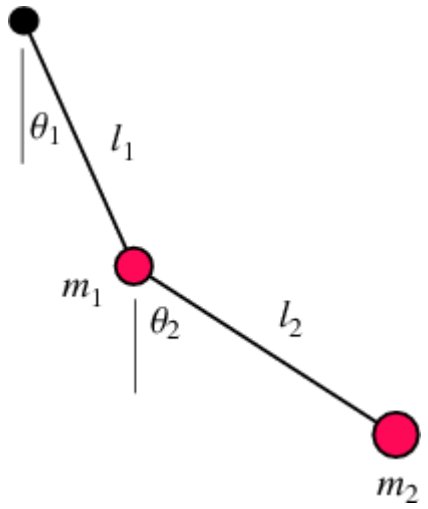

Figure 1: Coordinate measurements for the Lagrangian approach of solving the double pendulum.

$$L(q, \dot{q}, t) \equiv T(\dot{q}, t) - U(q, t)$$
$$\frac{\partial L}{\partial q} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}}$$

Where the dot notation indicates a derivative with respect to time. As shown in Figure 1, we have two coordinates for q: θ_1 and θ_2. To solve this system, we need the energies of each mass. This is most easily accomplished by using their x and y positions as such:

[1] http://scienceworld.wolfram.com/physics/DoublePendulum.html
[2] http://scienceworld.wolfram.com/physics/dimg270.gif

$$x_1 = l_1 \sin\theta_1$$
$$y_1 = -l_1 \cos\theta_1$$
$$x_2 = x_1 + l_2 \sin\theta_2 = l_1 \sin\theta_1 + l_2 \sin\theta_2$$
$$y_2 = y_1 - l_2 \cos\theta_2 = -l_1 \cos\theta_1 - l_2 \cos\theta_2$$

The potential energy U is simple in a gravitational field of strength g: $U = mgy$. Namely,

$$U = m_1 g y_1 + m_2 g y_2 = -m_1 g l_1 \cos\theta_1 - m_2(l_1 \cos\theta_1 + l_2 \cos\theta)$$

The kinetic energy may be written via its classical mechanics definition:

$$T = \frac{1}{2} m_1 (\dot{x_1}^2 + \dot{y_1}^2) + \frac{1}{2} m_2 (\dot{x_2}^2 + \dot{y_2}^2)$$

$$= \frac{1}{2} m_1 {l_1}^2 \dot{\theta_1}^2 + \frac{1}{2} m_2 \Big[{l_1}^2 \dot{\theta_1}^2 + {l_2}^2 \dot{\theta_2}^2 + 2 l_1 l_2 \dot{\theta_1} \dot{\theta_2} \cos(\theta_1 - \theta_2) \Big]$$

Thus, using the above definition of the Lagrangian, our system's Lagrangian is

$$L = \frac{1}{2}(m_1 + m_2) {l_1}^2 \dot{\theta_1}^2 + \frac{1}{2} m_2 {l_2}^2 \dot{\theta_2}^2 + m_2 l_1 l_2 \dot{\theta_1} \dot{\theta_2} \cos(\theta_1 - \theta_2) \tag{1}$$

Now, plugging this in for the Euler-Lagrange equations yields our two equations of motion for each mass:

$$(m_1 + m_2) l_1 \ddot{\theta_1} + m_2 l_2 \ddot{\theta_2} \cos(\theta_1 - \theta_2) + m_2 l_2 \dot{\theta_2}^2 \sin(\theta_1 - \theta_2) + g(m_1 + m_2) \sin\theta_1 = 0 \tag{2}$$

$$m_2 l_2 \ddot{\theta_2} + m_2 l_1 l_2 \ddot{\theta_1} \cos(\theta_1 \theta_2) - m_2 l_1 \dot{\theta_1}^2 \sin(\theta_1 - \theta_2) + m_2 g \sin\theta_2 = 0 \tag{3}$$

The solutions to these differential equations for θ_1 and θ_2 may be found numerically in the program to display realistic behavior.

1.3 Quantum Mechanics

The quantum mechanics project plans to demonstrate the quintessential hydrogen atom wavefunctions.
The most fundamental equation in (non-relativistic) quantum mechanics is the Schrödinger equation; once solved, you have the wave function and thereby everything there is to be known about the system. The Schrödinger equation reads

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) = \hat{H} \Psi(\vec{r}, t) \tag{4}$$

where Ψ is the wavefunction and $\hat{H}$ is the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r,t)$$

where m is the mass of the particle, ∇^2 is the Laplace operator, and $V(r,t)$ is the given potential.

We may solve this differential equation by assumption of form, guessing only one of many possible solutions, but then finding that these solutions are complete and combine to form the general solution. We assume the form

$$\Psi(\vec{r},t) = \psi(\vec{r})\phi(t)$$

We may plug this solution into the Schrödinger equation, and then divide by our assuming form for Ψ, resulting in

$$i\hbar\frac{1}{\phi}\frac{d\phi}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\nabla^2\psi + V$$

For our case, if we assume the potential depends only on r, then the two equations are separated; because they must always be equal, should we change one parameter e.g. t while holding the other constant, it must still be true; because r and t are independent however, this implies both sides of the equation are constant. We may write the time solution as

$$i\hbar\frac{1}{\phi}\frac{d\phi}{dt} = E$$

which has the solution

$$\phi(t) = e^{-iEt/\hbar} \tag{5}$$

We find that this constant E is actually the energy of the system, and for various Ψ_n, the nth excited state has energy E_n. We may construct our general wave function as a sum of these stationary states:

$$\Psi(\vec{r},t) = \sum c_n\psi_n e^{-iE_nt/\hbar} \tag{6}$$

Now, working on the spacial part, we must first specify a potential function; one of special interest (and the case which will be modeled by the project) is that of the Hydrogen atom, where the potential is the Coulomb potential between the electron and the proton nucleus:

$$V_H = \frac{1}{4\pi\epsilon_0}\frac{q_1q_2}{r} = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r}$$

where e is the elementary charge and ϵ_0 is the permittivity of free space. It is natural to use spherical coordinates for this system[3]; by using the spherical form of the Laplace operator, the Schrödinger equation reads

[3]NB: the convention for θ and ϕ are exchanged in standard physics notation in comparison to standard math notation i.e. ϕ is the azimuthal angle and θ the polar angle

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right]+V\psi=E\psi$$

Again, we attempt solving via separation of variables by looking for a spacial wavefunction in the form $\psi(r,\theta,\phi)=R(r)Y(\theta,\phi)$. If we plug this form in and divide by ψ as well as multiplying by a factor $-2mr^2/\hbar^2$ we get

$$\left\{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}\big[V(r)-E\big]\right\}+\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\}=0$$

The first term is a function only of r while the second is a function of only θ and ϕ. Like previously, these must each be constants, which we choose to write as such:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-\frac{2mr^2}{\hbar^2}\big[V(r)-E\big]=l(l+1)$$

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\}=-l(l+1)$$

To solve the angular equation first, we again try separation of variables with $Y(\theta,\phi)=\Theta(\theta)\Phi(\phi)$; plugging this in and dividing by Y gives us

$$\left\{\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right]+l(l+1)\sin^2\theta\right\}+\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=0$$

again indicating two individual pieces which are functions of only one variable, implying they are constant; this time they are set to be

$$\frac{1}{\Theta}\left[\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right]+l(l+1)\sin^2\theta=m^2$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=-m^2$$

The ϕ equation is simply solved:

$$\Phi(\phi)=e^{im\phi} \tag{7}$$

Where m may run negative to cover all possible solutions. The requirement that $\Phi(\phi+2\pi)=\Phi(\phi)$ is periodic limits m to integer values.

The θ equation has been solved to have the solution

$$\Theta(\theta)=AP_l^m(\cos\theta) \tag{8}$$

Where P_l^m is the associated Legendre function

$$P_l^m(x) \equiv (1-x^2)^{|m|/2}\Big(\frac{d}{dx}\Big)^{|m|}P_l(x)$$

where $P_l(x)$ is the lth Legendre polynomial

$$P_l(x) \equiv \frac{1}{2^l l!}\Big(\frac{d}{dx}\Big)^l (x^2-l)^l$$

both of which are, in our case, functions of $\cos\theta$ i.e. $x = \cos\theta$. There are two other solutions (because the differential equation is second order) however they are unphysical, and thus ignored. Because the total probability must be 1, we need to normalize the wavefunction, which is done convieniently for each piece separately. Doing this, we end up with our final answer for Y:

$$Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta) \tag{9}$$

where $\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m \leq 0$. These are notably the **spherical harmonics**.

For solving the radial equation, it is convenient to make the substitution $u(r) \equiv rR(r)$ (and thus $dR/dr = rd^2u/dr^2$; doing so and plugging in our Coulomb potential for the hydrogen atom gives us

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

This is solved by looking at the asymptotic behaviors of u and introducing some extra functions to create the in-between behavior. We introduce $\kappa \equiv \frac{\sqrt{-2mE}}{\hbar}$ (which is real, since bound state energies are negative and the electron is bound) and $\rho \equiv \kappa r$ and $\rho_0 \equiv \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$. We introduce the "helper" function $v(\rho)$ and find that the radial equation now reads

$$\rho\frac{d^2v}{d\rho^2} + 2(l+1-p)\frac{dv}{d\rho} + \big[\rho_0 - 2(l+1)\big]v = 0$$

We try expressing $v(\rho)$ as a power series and using the derivatives find that the coefficients are determined by a recursive formula. We also find that the series must terminate after some maximal index number j_{max} because if it didn't we'd get unphysical results ($u(\rho) as an exponential of \rho$). Defining the principal quantum number

$$n \equiv j_{max} + l + 1$$

we determine ρ_0 and thereby the energies:

$$E_n = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} \tag{10}$$

and finally our radial function

$$R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}v(p) \tag{11}$$

where $v(p)$ is a polynomial of degree j_{max} whose coefficients are determined by the recursive formula

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}c_j$$

and thus we have finally solved for the constituent pieces of the stationary states of our wavefunction. Because they are orthogonal and complete, being careful of normalization we may use linear combinations of them to build whatever wavefunction we like, in a manner exactly like Fourier analysis. More explicitly, the spacial term is

$$\psi_{nlm} - \sqrt{\Big(\frac{2}{na}\Big)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}}e^{-r/na}\Big(\frac{2r}{na}\Big)^l \Big[L^{2l+1}_{n-l-1}(2r/na)\Big]Y_l^m(\theta,\phi) \tag{12}$$

where

$$L^p_{q-p}(x) \equiv (-l)^p\Big(\frac{d}{dx}\Big)^p L_q(x)$$

$$L_q(x) \equiv e^x\Big(\frac{d}{dx}\Big)^q(e^{-x}x^q)$$

and a is the Bohr radius $a = (r\pi\epsilon_0\hbar^2)/(me^2)$.

1.4 Thermal and Statistical Physics

The thermal and statistical physics project simulates a gas in a box i.e. the interaction of many particles in an enclosed space.
The goal of these areas of physics is to model the behavior of large collections of particles (order 10^{20} or larger). Because of the nature of the program, most equations won't hold because they are made with approximations based on the fact that the number of particles N is very large. However, one relevant equation is the simple yet fundamental equation for conservation of momentum

$$\sum_i^N \vec{p}_{i,i} = \sum_j^N \vec{p}_{j,f} \text{ when } \frac{d\vec{P}}{dt} = 0 \tag{13}$$

which says that when there are no external forces ($\vec{F}_{net} \equiv d\vec{P}/dt$, where P is the total momentum), the momentum of the system will be conserved. This applies to the collision of particles, meaning that their total momentum remains unchanged by a collision (Newton's Third Law says no net force is exerted on either due to each other). Thus, though they bounce in different directions, knowing their momenta must have the same vector sum before and after allows

us to solve for their final individual momenta. Also necessary (if the given parameters do not suffice) is conservation of energy:

$$\sum_{i}^{N} \frac{1}{2} m_i v_{i,i}^2 = \sum_{j}^{N} \frac{1}{2} m_j v_{j,f}^2 \tag{14}$$

which says that the total (kinetic, as we have no potential) energy of the system remains constant. This holds true as long as the collisions are elastic (no internal force or energy changes to hold them together) and no net force acts on the system. It is somewhat redundant, as because $\vec{p} = m\vec{v}$ for particles of constant mass, $E = \frac{p^2}{2m}$, so if momentum is conserved then energy would be as well. However the extra equation constrains more parameters, should we need them, to solve for the final state of the system after a collision.

2 Goals

The overall project should be self-contained in the sense that the user may navigate the programs and back through some "hub" without explicitly having to run separate files. Each sub-project should be interactive and display a physical system in some realistic capacity. Below are the individual goals for each sub-project:

2.1 Kinematics

- Allow the user to pick mass, radius, velocity (or choose them to be random) for the launched object.
- Draw the launched object in a field and show the path of motion it travels
- Possibly add external forces e.g. winds, drags that will alter the motion in some more complex manner

2.2 Chaos Theory

- Allow the user to enter masses and lengths of the pendula, as well as initial angles.
- Go beyond the double pendulum into a triple pendulum and possibly even an n-pendulum system.

2.3 Quantum Mechanics

- Allow the user to enter the quantum numbers to view different eigenstates of the hydrogen atom.
- Display either the wave function or the probability density for each state

2.4 Thermal and Statistical Physics

- Have realistic particle bounce which obeys the laws of physics
- Allow user some input such as average velocity of particles or number of particles
- Implement some method of displaying average characteristics of the particles, which is the point of this discipline

3 Methods

This program will be written entirely in Python using primarily the VPython library for the graphics, but also using some mathematical libraries such as NumPy. The files will be separate but navigable via either the terminal or (more preferably) the actual window in which the simulation is displayed, so that running the main file will allow you to examine all of the files.
VPython has plenty of resources available to make these projects possible; the ease of creating mutable objects leaves most of the work into simply efficiently coding the math in. For example, the double pendulum program is made much simpler through frames and $.rotate(\theta)$ methods. VPython was built for physics simulations, which means it is the perfect platform for my project.
Currently, a simple kinematics program has been finished, and a particle bounce system with two particles has been built (but realistic bounce between particles not yet implemented). A rudimentary system of navigating the files through the terminal causes the current program to be halted, and a new scene drawn with the imported program, which simulates execution of another file.