PELEG BAR SAPIR

PHYSICS SIMULATIONS (LECTURE NOTES)

1

Introduction

1.1 Why are Simulations Used?

Text

1.2 Python

1.2.1 General

Text

1.2.2 NumPy

Text

1.3 A Bit About Git

Text

1.4 Some Mathematical Background

1.4.1 Radians

In the context of trigonometry in mathematics and physics, we most commonly use **radians** in place of **degrees**. This sometimes causes some confusion with newer students, so I find it appropriate to briefly discuss the what and why of radians and their usage.

Degrees are defined as a measurement of **angles**. That is, for historical and practical reasons we define a full rotation as 360°. The main problem with using angles is that they are units by themselves, i.e. they differ from lengths. This can cause some consistency issues with regards to units. Consider for example the following equation for a **centripetal force**:

$$F = m\frac{v^2}{r}, \tag{1.1}$$

where m is the mass of the rotationg object, v^2 is the square of the linear velocity the object experiences in each time instance, and r is the distance of the rotating object from the center of rotation (Figure 1.1).

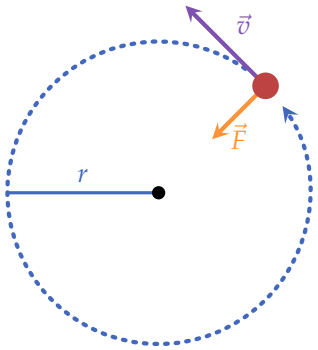

Figure 1.1: Object with mass m in perfect cicular motion with distance r around a central point. The force acting on the object is directed towards the center and has value $F = m\frac{v^2}{r}$.

In the standard SI scheme, F has units of $[\mathrm{N}]$ ("Newtons"), i.e. $\left[\mathrm{kg\,m\,s^{-1}}\right]$. We know that m has units of $[\mathrm{kg}]$, v of $\left[\mathrm{m\,s^{-1}}\right]$ and r units of $[\mathrm{m}]$ - so both sides of the equation have the same units.

However, nothing prevents us from measuring the rotation associated with $\frac{v^2}{r}$ directly using angular velocity ω - which can be defined as the amounth of degrees of rotation per time T if the rotation is uniform:

$$\omega = \frac{\theta}{T}, \tag{1.2}$$

or more generally as the time derivative of the angle,

$$\omega = \frac{\mathrm{d}\theta}{\mathrm{d}t} = \dot{\theta}. \tag{1.3}$$

If we measure the angle θ in degrees, we get that the units of angular velocity is $\left[^\circ\,\mathrm{s^{-1}}\right]$. If we then want to use ω in the centripetal force equation, we must somehow cancel the degrees unit to get the proper units of $[\mathrm{N}]$. This obviously leads to a somewhat cumbersome equation.

A much better approach is to measure the *ratio* between the length of an arc created by our angle at a radius R and the same radius itself (Figure 1.2). This gives a unitless measure which we call *radians*, and can be either ignored in the unit calculation (since it is unitless), or simply denoted $[\mathrm{rad}]$.

Another way to view radians is that they measure an arc length in units of the radius (not necessarily a unit radius). If we scale the radius by any scalar, an arc length of the same angle will scale by exactly the same scalar, and so the amount of radians we measure for the arc length won't change (the ratio stays the same, as both the numerator and denominator are scaled by the same number).

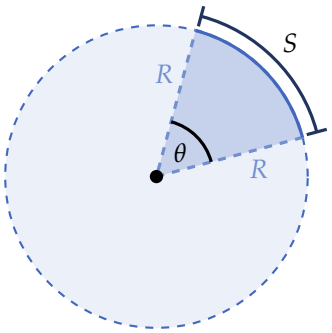

Figure 1.2: Measuring angles using radians. We express the length of S in units of R, e.g. if $S = 1$ then the arc length is equal to R, if $S = \pi$ the arc length is half that of the entire circumference of the circle, etc. The ratio S/R is constant for any real positive value of R, and thus can be used to uniquely describe the angle θ.

We can easily replace any measurement of angles in degrees by a corresponding measurement in radians, since any amount of degrees has a 1-to-1 correspondence with a single value in radians. Let us find this correspondence: since there are 2π radii in a full circle, and a full angle is $360°$, we see that each radii length of an arc corresponds to $\frac{360°}{2\pi} = \frac{180°}{\pi} \approx 57.2958°$.

Now, using the radian unit to measure an angle θ, we get that ω has units of $\left[\text{rad}\,\text{s}^{-1}\right]$, or simply $\left[\text{s}^{-1}\right]$. In turn, if we raise ω to the 2nd power and multiply it by the distance r between the rotating object and center of rotation, and the mass m of the object, we get the units $\left[\text{kg}\,\text{m}\,\text{s}^{-1}\right]$, which is exactly the excplicit form of Newtons. Indeed, using this perspective, Equation 1.1 can be written as

$$F = m\omega^2 r. \tag{1.4}$$

In my mind, this is simply beautiful.

Let's finish with some example correspondences between degrees and radians, which can be seen in Table 1.1 below.

[°]	[rad]
0	0
30	$\frac{\pi}{6}$
45	$\frac{\pi}{4}$
60	$\frac{\pi}{3}$
90	$\frac{\pi}{2}$
120	$\frac{2\pi}{3}$
180	π
270	$\frac{3\pi}{2}$
360	2π

Table 1.1: Example correspondences between measurements in degrees and radians.

1.4.2 *Taylor Series*

For some functions, it is rather easy to calculate their values at some point x_0: for example, given a polynomial function

$$P(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_n x^n, \tag{1.5}$$

it is rather easy to calculate its value at any real point x: all the operations that we need to use are addition and multiplication of real numbers, and raising real numbers to an integer power (which in principle can be implemented as repeated multiplications). Modern computers calculate such operations at the rate of billions of times a second.

Note 1.1 Floating point representation

For the sake of simplicity, I'm ignoring the entire topic of floating point numbers and relevant questions of precision.

Example 1.1 Calculating a value of a simple polynomial

Given the polynomial $P(x) = 3x^2 - 2x + 7$, we can easily calculate its value at, say, $x = 5$:

$$P(x = 5) = 3 \cdot 5^2 - 2 \cdot 5 + 7 = 3 \cdot 25 - 10 + 7 = 72.$$

For other functions, on the other hand, it is not that easy to calculate their values at most points. For example, consider the exponential function $f(x) = e^x$. We know precisely exactly one real value of the function: at $x = 0$, the function returns 1. But for any other value of x, we don't really know the value of the function. That is, we know all values *symbolicaly* (for example, $f(1) = e$, $f(2) = e^2$, etc.) - but not in explicit form.

However, given that the function behaves nicely enough (we'll discuss in a moment what that means), we can *approximate* its value to whatever percision we wish, using a method called the **Taylor series** of the function. The "price" we pay for greater percision is simply performing more calculations.

The basic idea of a Taylor series of a function $f(x)$ is that we approximate the function by adding higher and higher derivatives of the same function, at some point a for which we know precisely the value of the function and its derivatives to any order. This might sound a bit abstract, so let's explore this process using an example function - again, the exponential $f(x) = e^x$. As mentioned, we only really know one value of the function precisely, namely at $a = 0$: $e^0 = 1$.

We can therefore start approximating e^x simply as e^0. This is obviously a very impercise approximation, but the important thing

is that if we look at a very close neighborhood of $x = 0$, the approximation is not *that* bad: consider, for example $x_0 = 0.0001$. Our approximation gives $e^{x_0} \approx 1$, which is not far from the more precise value $e^{x_0} = 1.000100005$ (the value here is shown up to the ninth decimal). Of course, the closer we get to $a = 0$, the better our approximation gets: for example, with $x_1 = 0.00001$, we get $e^{x_1} \approx 1$ again, where in reality $e^{x_1} = 1.000010000$ (also shown here up to the ninth decimal). On the other hand, if we as we get farther away from $x = 0$, the approximation becomes worse and worse, as seen in Table 1.2 below.

x	e^x (exact)	Δ (error)
0.000	1.000000000	0.000000000
0.001	1.001000500	0.001000500
0.010	1.010050167	0.010050167
0.100	1.105170918	0.105170918
0.500	1.648721271	0.648721271
0.510	1.665291195	0.665291195
0.520	1.682027650	0.682027650
1.000	2.718281828	1.718281828
1.100	3.004166024	2.004166024
1.500	4.481689070	3.481689070
2.000	7.389056099	6.389056099

Table 1.2: Zero order Taylor series approximation of e^x.

Now, let's take this a step further: since the derivative of a function at a point tells us how the functions changes close to the point, we can use this information to improve our approximation by adding the value of the first derivative of e^x at $x = 0$, which is also 1. In fact, this is true for any order derivative of e^x, since $\frac{d^n}{dx^n} e^x = e^x$ for any $n \in \mathbb{N}$. Since the derivative changes with the value of x, we will multiply it by x in the approximation. Thus we get

$$e^x \approx 1 + 1 \cdot x = 1 + x, \tag{1.6}$$

which we call the **first order** approximation of the function e^x. Table 1.3 below shows the same values from Table 1.2 for x, but using the first order approximation for e^x.

By examining Table 1.3 it's clear that $1 + x$ is a much better approximation for e^x than just 1. Of course, we can take a further step: the second derivative of a function at a point tells us how the change in the function itself changes around that point. We can take the second derivative of e^x (which is by itslef e^x), again substitute $x = 0$, get $e^0 = 1$, and use this with x^2 to apperoximate e^x even better. In fact, let's already take this idea to its logical conclusion: we'll simply use the infinite power series in x, i.e. $1, x, x^2, x^3, \ldots, x^n, \ldots$

x	$1+x$	e^x (exact)	Δ (error)
0.000	1.000000000	1.000000000	0.000000000
0.001	1.001000000	1.001000500	0.000000500
0.010	1.010000000	1.010050167	0.000050167
0.100	1.100000000	1.105170918	0.005170918
0.500	1.500000000	1.648721271	0.148721271
0.510	1.510000000	1.665291195	0.155291195
0.520	1.520000000	1.682027650	0.162027650
1.000	2.000000000	2.718281828	0.718281828
1.100	2.100000000	3.004166024	0.904166024
1.500	2.500000000	4.481689070	1.981689070
2.000	3.000000000	7.389056099	4.389056099

Table 1.3: First order Taylor series approximation of e^x.

and attach to each x^k the value given by $\frac{d^n}{dx^n}e^x\Big|_{x=0} = 1$, so we get

$$e^x \approx 1 + x + x^2 + x^3 + \cdots + x^n + \cdots = \sum_{n=0}^{\infty} x^n. \tag{1.7}$$

This, however doesn't quite work. The coefficients of each term have to be adjusted. By assuming that at the limit where $n \to \infty$ the approximation should be with zero error, we get that for each n,

$$\frac{d^n}{dx^n}e^x = \frac{d^n}{dx^n}\left(1 + x + x^2 + \ldots\right) \equiv s(x). \tag{1.8}$$

Calculating the general n-th derivative of Equation 1.7 is rather easy. Let's examine the case for $n = 3$: the first three derivatives of Equation 1.7 are

$$\begin{aligned}
\tfrac{d}{dx}s(x) &= 1 + 2x + 3x^2 + 4x^3 + \ldots, \\
\tfrac{d^2}{dx^2}s(x) &= 2 + 6x + 12x^2 + \ldots, \\
\tfrac{d^3}{dx^3}s(x) &= 6 + 24x + \ldots,
\end{aligned}$$

and if we subtitute $x = 0$ we get

2

Thermodynamics

2.1 *Preface*

Text text text

2.2 *Ideal gas*

2.2.1 *Theory*

There are several commonly used models for the behaviour of gasses. A very simple yet powerful one is the **ideal gas** model: it describes gas particles as being perfect spheres which move around in an enclosed container and undergo elastic collisions with other particles and the walls of the container. In common conditions such as atmospheric pressure and temperatures around 300 [K], gasses such as helium (He), argon (Ar), nitrogen (N_2), oxygen (O_2) and carbon dioxide (CO_2) behave like ideal gasses (assuming no chemical reations take place). However, the ideal gas model fails under high pressures, low temperatures, chemical interactions and some physical processes such as adsorption or multipolar interactions.

The principle equation describing an ideal gas is the **ideal gas law**:

$$PV = nRT, \tag{2.1}$$

where (SI units in parentheses):

- P is the pressure of the gas (Pa),
- V is the volume of the container (m^3),
- n is the amount of gas (mol),
- R is the **gas constant**, $R = 8.314 \left[\mathrm{J\,K^{-1}\,mol^{-1}}\right]$, and

- T is the temperature of the gas (K).

Maxwell-Boltzman distribution

Mean free path

Temperature from energy

2.2.2 *Simulating an ideal gas using perfectly elastic spheres*

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Sphere-wall collision

An elastic collision between a particle and a wall causes the particle's velocity to flip in the direction of the wall's normal (Figure 2.1).

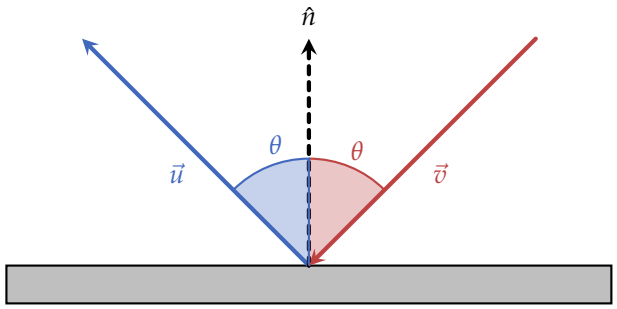

Figure 2.1: Collision of a particle and a wall. The particle bounces in such a way that the component of its velocity $\vec{v}$ in the direction of the wall's normal $\hat{n}$ is flipped. The resulting velocity $\vec{u}$ has the same angle to $\hat{n}$ as $\vec{v}$ does.

The component of $\vec{v}$ in the direction of $\hat{n}$ is

$$\vec{v}_{\parallel} = \langle \vec{v} | \hat{n} \rangle \, \hat{n}. \tag{2.2}$$

Therefore, the component of $\vec{v}$ orthogonal to $\hat{n}$ is

$$\vec{v}_{\perp} = \vec{v} - \vec{v}_{\parallel} = \vec{v} - \langle \vec{v} | \hat{n} \rangle \, \hat{n}. \tag{2.3}$$

In the case of $\vec{u}$, the orthogonal component is the same as that of $\vec{v}$, but the parallel component is inverted:

$$\begin{aligned} \vec{u}_{\perp} &= \vec{v}_{\perp}, \\ \vec{u}_{\parallel} &= -\vec{v}_{\parallel}. \end{aligned} \tag{2.4}$$

and altogether we get

$$\begin{aligned} \vec{u} &= \vec{u}_{\perp} + \vec{u}_{\parallel} \\ &= \vec{v} - \langle \vec{v} | \hat{n} \rangle \, \hat{n} - \langle \vec{v} | \hat{n} \rangle \, \hat{n} \\ &= \vec{v} - 2 \langle \vec{v} | \hat{n} \rangle \, \hat{n}. \end{aligned} \tag{2.5}$$

Example 2.1 A simple sanity check

To make a simple validation of this equation, let's examine the case for a collision with a wall which is oriented in the xy-plane (i.e. its normal points in the z-direction): given the

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velocity $\vec{v} = \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix}$, Equation 2.5 becomes

$$\begin{aligned}
\vec{u} &= \vec{v} - 2\langle \vec{v} | \hat{n} \rangle \hat{n} \\
&= \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} - 2 \left\langle \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} \middle\| \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\rangle \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \\
&= \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} - 2(\cancel{v_x \cdot 0} + \cancel{v_y \cdot 0} + v_z \cdot 1) \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \\
&= \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} - 2v_z \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \\
&= \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} - 2 \begin{bmatrix} 0 \\ 0 \\ v_z \end{bmatrix} \\
&= \begin{bmatrix} v_x \\ v_y \\ v_z \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ -2v_z \end{bmatrix} \\
&= \begin{bmatrix} v_x \\ v_y \\ -v_z \end{bmatrix},
\end{aligned}$$

as expected.

Note 2.1 BLA

The reader is encouraged to repeat the above calculation for the cases of walls oriented in the xz- and yz-planes.

sphere-sphere collision

Consider two solid spheres which have a single point of contact $\boldsymbol{A}$. Let $m_1, r_1, \vec{x}_1$ and $\vec{v}_1$ be the mass, radius, position and velocity of the first sphere, and $m_2, r_2, \vec{x}_2$ and $\vec{v}_2$ the respective quantities for the second sphere (Figure 2.2). The line connecting the centers of the two spheres is in the direction $\hat{n}$ (without loss of generality let us assume that the normal vector $\hat{n}$ points from $\vec{x}_1$ towards $\vec{x}_2$). The unit vector $\hat{t}$ is orthogonal to $\hat{n}$ (and without loss of generality we will assume that it is oriented counter-clockwise from $\hat{n}$).

Note that we did not define a coordinate system, nor the number

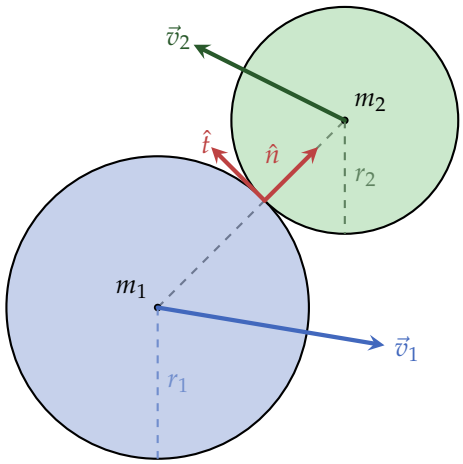

Figure 2.2: Text text text

of dimensions d for the problem. The only restriction is that $d \geq 2$.

Conservation of momentum means that the velocities of the spheres following the collision, $\vec{u}_1, \vec{u}_2$, are related to their velocities before the collision by

$$\begin{aligned} & m_1\vec{v}_1 + m_2\vec{v}_2 = m_1\vec{u}_1 + m_2\vec{u}_2 \\ \Rightarrow \quad & m_1\left(\vec{v}_1 - \vec{u}_1\right) = m_2\left(\vec{u}_2 - \vec{v}_2\right). \end{aligned} \tag{2.6}$$

Conservation of energy means that the velocities are also related by

$$\begin{aligned} & \frac{1}{2}m_1\|\vec{v}_1\|^2 + \frac{1}{2}m_2\|\vec{v}_2\|^2 = \frac{1}{2}m_1\|\vec{u}_1\|^2 + \frac{1}{2}m_2\|\vec{u}_2\|^2 \\ \Rightarrow \quad & m_1\left(\|\vec{v}_1\|^2 - \|\vec{u}_1\|^2\right) = m_2\left(\|\vec{u}_2\|^2 - \|\vec{v}_2\|^2\right). \end{aligned} \tag{2.7}$$

However, the forces involved in the collision can not have a component in the $\hat{t}$ direction, and are limited to only point in the $\hat{n}$ direction. Therefore, we can reduce the problem to this direction only by projecting all velocities involved in the problem on $\hat{n}$, i.e. Equation 2.6 becomes

$$m_1\langle\vec{v}_1|\hat{n}\rangle + m_2\langle\vec{v}_2|\hat{n}\rangle = m_1\langle\vec{u}_1|\hat{n}\rangle + m_2\langle\vec{u}_2|\hat{n}\rangle. \tag{2.8}$$

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$$\begin{aligned} \vec{u}_1 &= \vec{v}_1 - \frac{2m_2}{m_1+m_2}\langle\vec{v}_1 - \vec{v}_2|\hat{n}\rangle\,\hat{n}, \\ \vec{u}_2 &= \vec{v}_2 + \frac{2m_1}{m_1+m_2}\langle\vec{v}_1 - \vec{v}_2|\hat{n}\rangle\,\hat{n}. \end{aligned} \tag{2.9}$$

To avoid reduntant calculations, we can factor out the common quantity of both velocities:

$$K = \frac{2}{m_1+m_2}\langle\vec{v}_1 - \vec{v}_2|\hat{n}\rangle\,\hat{n}, \tag{2.10}$$

yielding

$$\begin{aligned} \vec{u}_1 &= \vec{v}_1 - Km_2, \\ \vec{u}_2 &= \vec{v}_2 + Km_1. \end{aligned} \tag{2.11}$$

Reducing collision test complexity

2.3 Brownian dynamics