AST2000 - Part 1
Modelling a Rocket Engine

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We have successfully modelled a rocket engine by studying essential statistical physics and simulating the processes that happen inside its combustion chamber. From learning more about these processes we were able to determine that we would need to bring circa 45 000 kg fuel on our journey in order for an eventual launch to be successful, as well as the magnitude of our rocket's thrust force. We were able to simulate a launch and compare our results with those that our research team calculated, and found that all went great, except for a slight deviation in our expected position.

I. INTRODUCTION

In this study we aim to learn more about statistical physics in order to simulate the behavior of gas particles within the combustion chamber of a rocket, and use this to accurately model our own rocket's engine. We will eventually use the results from our simulations and our newfound knowledge of statistical physics in order to simulate a launch from our home planet Doofenshmirtz. In further studies, we will take good use of what we learn here, as we'll eventually unveil incredibly interesting information about our solar system and the planets within it. We'll further advance our rocket's on-board software, launch our rocket, and eventually travel towards and land on one of our solar system's more habitable planets.

II. THEORY

We will first focus on the rocket engine itself. The main principle here is that we have a large amount of gas particles moving through and out of the engine's combustion chamber at all times. As these particles exit the chamber, our rocket is propelled forward because of the conservation of momentum. These gas particles all have different velocities that are impossible to know for sure, and we therefore need to use both the *Gaussian Distribution* and the *Maxwell-Boltzmann Distribution* in order to describe this.

The normal probability distribution can be defined as

$$f(\mu, \sigma, x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \tag{1}$$

where μ is the mean value in the interval we want to look at values of x for, and σ is the *standard deviation.* This is defined as

$$\sigma = \frac{\text{FWHM}}{\sqrt{8\ln 2}} \tag{2}$$

Where FWHM is the *Full Width at Half Maximum* (see Appendix A). This is a measure of the symmetrical Gaussian Distribution curve's width at half its maximum value.

If we want to find the probability P of a particle residing within an interval $a \leq x \leq b$, we integrate this expression in the following way:

$$P(a \leq x \leq b) = \int_a^b f(\mu, \sigma, x)dx \tag{3}$$

From Lecture Notes 1A [1], we know that we then get the common expression for the Gaussian Distribution:

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{4}$$

The Gaussian Distribution can also be used to find the probability of a particle's velocity components v_x, v_y and v_z residing within a given interval. The constructed curve describing the probability distribution will be symmetrical, and the mean μ will be zero. This means that for every gas particle having a velocity component v_x giving it momentum p_x, there necessarily is also a gas particle having the velocity component $-v_x$ giving it the momentum $-p_x$ in the same gas. From Lecture Notes 1A [1] we know that the Gaussian probability distribution for the particles' velocity components can be calculated using

$$\begin{aligned} P(v_x) &= \frac{1}{\sqrt{2\pi}\sigma} e^{-v_x^2/(2\sigma^2)} \\ P(v_y) &= \frac{1}{\sqrt{2\pi}\sigma} e^{-v_y^2/(2\sigma^2)} \\ P(v_z) &= \frac{1}{\sqrt{2\pi}\sigma} e^{-v_z^2/(2\sigma^2)} \end{aligned} \tag{5}$$

which in fact is the Maxwell-Boltzmann Distribution on a vectorized form. The standard deviation is then defined as

$$\sigma = \sqrt{\frac{kT}{m_{\text{H}_2}}} \tag{6}$$

If we want to look at the absolute value of the particles' velocities, this is no longer a symmetric Gaussian distribution. This immediately follows from the fact that the absolute velocity cannot be negative, as it's defined as

$$v = \sqrt{v_x^2 + v_y^2 + v_z^2} \tag{7}$$

We will assume that the rocket engine's fuel tanks are equipped only with pure H_2 gas, and that this can be approximated as an ideal gas. Following this assumption, we once again know from Lecture Notes 1A [1] that the probability of a particle's absolute velocity residing within an interval $[v, v + dv]$ is given by the Maxwell-Boltzmann distribution for absolute velocity

$$P(v)dv = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}} 4\pi v^2 dv \tag{8}$$

When the gas temperature is T, m is the mass of the atoms in the gas, and k is defined as the Boltzmann constant. We can use (8) to derive the following expression for the mean absolute velocity $\langle v\rangle$ of a particle in a gas with this temperature and mass (see Appendix B):

$$\langle v\rangle = \sqrt{\frac{8kT}{m\pi}} \tag{9}$$

In turn, this gives us an expression for the mean energy of the particles in an ideal gas (see Appendix D):

$$\langle E\rangle = \frac{3}{2}kT \tag{10}$$

III. METHOD

Before we begin modelling our rocket's engine, we have to test our simulation software to see if it's realistic. To do this, we will first check if it's able to use (A1) and (3) to correctly calculate the probability of a particle residing within the intervals

$$\begin{aligned} -1\sigma \leq & x - \mu \leq 1\sigma \\ -2\sigma \leq & x - \mu \leq 2\sigma \\ -3\sigma \leq & x - \mu \leq 3\sigma \end{aligned}$$

with the expected probabilities being

$$\begin{aligned} \pm 1\sigma &: 68\% \\ \pm 2\sigma &: 95\% \\ \pm 3\sigma &: 99.7\% \end{aligned}$$

We will further study the difference between the Gaussian and the Maxwell-Boltzmann probability distributions by letting our particles' velocity component v_x exist within the interval

$$v_x \in [-2.5 \times 10^4,\ 2.5 \times 10^4] \text{ m/s}$$

and then let our software calculate the probability distribution using the Gaussian Distribution (A1). It'll then use (3) to integrate over the distribution in the interval

$$5 \times 10^3 \text{ m/s} \leq v_x \leq 30 \times 10^3 \text{ m/s}$$

to calculate the probability of a particle's v_x component existing within this interval, in order to see if our integrator works as expected. Furthermore, we want to calculate the probability distribution of the particle's absolute velocity v when we let it exist within the interval

$$v \in [0,\ 3 \times 10^4] \text{ m/s}$$

When our software performs these calculations, we will let the gas contain 100 000 particles, and its temperature be 3000 Kelvins.

We'll plot our software's calculated probability distribution data to see if the curves look as expected. If our software succeeds in calculating reasonable data, as well as the probabilities mentioned at the beginning of this section, it affirms its reliability when we will simulate the energetic gas within our rocket's engine.

After testing our software, we will begin modelling our rocket's engine. In order for us to do this, we will first have to invoke a few more assumptions and simplifications:

- The temperature and amount of particles within the gas is constant inside the combustion chamber at all times.
- Gravitational effects are negligible when simulating the processes inside the chamber.
- We will ignore the possibility of particle collisions.
- When a particle collides with one of the walls of the chamber, the collision is completely elastic.

We will divide the engine's combustion chamber into multiple small boxes with cross-sectional areas of 10^{-12} m^2 each. Our research team at the University of Oslo informed us that the cross-sectional area of our spacecraft is 16 m^2, which means that we'll need a total of 16×10^{12} gas boxes in order to cover the entire bottom of the rocket and make up the engine. We will begin by simulating the energetic gas within one of these boxes, both with the box being comprised of 100 and 100 000 gas particles. We let the gas particles' initial positions at the beginning of the simulations be uniformly distributed throughout the gas box, and update their positions by multiplying their respective velocities with the length of a time step. We let the simulations run for one nanosecond each, and we have a thousand time steps, meaning the time between each update of the particles' positions are 10^{-12} seconds. The particles' initial velocity components are distributed using the Gaussian probability distribution as defined in (5), by letting the mean μ be zero, and the standard deviation be as defined in (6).

During the simulation we'll count each time a particle collides with one of the walls within the box, as we then need to redirect their velocity component component that is orthogonal to the wall they collide with. Since the collisions are assumed to be elastic, this component will then point in the opposite direction, but be the same in magnitude. We want to see if our simulations are realistic, and to do this we will calculate the mean kinetic energy of the gas particles at the end of the collision, be iterating over all of them in the following way:

$$\langle E\rangle_{\text{numerical}} = \sum_{i=0}^{N} \frac{1}{2} m_{\text{H}_2} v_i^2 \tag{11}$$

Since ideal gases don't have intermolecular forces and we therefore don't need to include any potential energy contributions. We will then compare these results to the analytical expression for calculating the mean energy of a particle in an ideal gas (see Appendix D):

$$\langle E\rangle_{\text{analytical}} = \frac{3}{2} kT \tag{12}$$

If the results are reasonable in comparison, this is another confirmation of our software being reliable.

After looking at how the energetic gas behaves inside an enclosed box, we'll add nozzles to each of the gas boxes and simulate the gases once again to see how many particles exit the combustion chamber every second. We imagine that the gas boxes that make up the combustion chamber each have a nozzle located right in the middle at the bottom of them with an area of 0.25×10^{-12} m^2. We need to check for each particle if it exits the box at each time step throughout the simulation, and if so, respawn a new particle in the box with a random position and velocity, as the number of particles present in the box has to be constant at all times. We'll do this by checking whether or not a particle's x- and y-coordinates are within the hole that makes up the nozzle, and if its z-coordinate surpasses the bottom of the box. We'll count each time a particle exits, and use this to calculate how much mass the box loses per second:

$$mlr_{\text{box}} = m_{\text{H}_2} pps \tag{13}$$

Where mlr_{box} is the box's mass loss rate, and pps is the amount of particles exiting the box per second.

We will calculate the thrust force exerted by the box during the simulation in the following way:

$$f_{\text{box}} = \frac{1}{N_{\text{s}}} \sum_{i=0}^{N_{\text{s}}} \sum_{j=0}^{N_{\text{p}}} m_{\text{H}_2} \frac{|v_{z,j}|}{\Delta t} \tag{14}$$

Where N_{s} is the amount of time steps in the simulation, and N_{p} is the amount of particles that exit at the i^{th} time step. We define $v_{z,j}$ is the j^{th} particle's velocity in the z-direction, which propels the rocket upward, and Δt is the length of one time step in the simulation. By assuming that mlr_{box} and f_{box} is equal for all boxes, we can multiply these values by the amount of boxes to find the engine's total mass loss rate mlr and thrust force f.

Before we simulate our first rocket launch, we wish to test our engine's performance by making it perform an arbitrary boost Δv that we think is realistic when considering how much we'll need to accelerate it during an actual launch. When performing this boost we will ignore gravity, which of course is a major simplification as our rocket will be accelerated in the opposite direction of the gravitational force during an actual launch. This simulation is more to help us see how much fuel our rocket would use during the boost itself, and how much thrust force it exerts in this time period. We can do this by approximating the rocket's acceleration as constant during the simulation. We define it as

$$a = \frac{f}{m} \tag{15}$$

Where f is the thrust force our engine exerts in one second, and m is the total mass of the rocket. This includes its fuel and the mass of the spacecraft itself, which is 1100 kg. From (15), we can find the amount of time it takes for our rocket to accelerate from zero to Δv:

$$\Delta t = \frac{a}{\Delta v} \tag{16}$$

Which lets us calculate the engine's total fuel consumption during the boost:

$$\Delta m = mlr_{\text{box}} N_{\text{box}} \Delta t \tag{17}$$

where N_{box} is the amount of boxes that make up the engine. We also find the total thrust force exerted:

$$F = f \Delta t \tag{18}$$

After studying the amount of fuel consumed and thrust exerted during the arbitrary boost Δv, we can further decide if we need to include less or more fuel for our launch simulations. If we want to increase our thrust force, we can also attempt to increase the amount of gas particles in each box. We plan to keep the temperature of the gas contained in the combustion chamber at 3000 Kelvins, since this is the most realistic. We'll then start by simulating a rocket launch from our home planet Doofenshmirtz' frame of reference. To do this, our simulation software uses the leap frog integration method, which works in the following way

$$\begin{aligned} v_h &= v_i + a_i \frac{\Delta t}{2} \\ r_{i+1} &= r_i + v_h \Delta t \\ v_{i+1} &= v_h + a_{i+1} \frac{\Delta t}{2} \end{aligned}$$

Where a, v and r are the rocket's acceleration, velocity and position vectors, and Δt is the length of each time step in the simulation. Previously we used $\Delta t = 10^{-12}$s since the gas box simulations only lasted for one nanosecond, but the simulated rocket launch may last up to 20 minutes, and we therefore choose to initially simulate the rocket launch with $\Delta t = 1$s, though we may need to change this.

To calculate the rocket's acceleration a, we now need to take account for gravitational pull of our home planet as well. We will ignore the air resistance, as this is minuscule compared to the gravitational pull and rocket's thrust

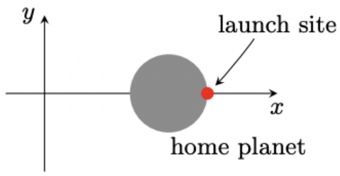


Figure 1. Our spacecraft's launch position on the surface of Doofenshmirtz

force. We define the acceleration in the following way using Newton's 2^{nd} law:

$$\begin{aligned} a &= \frac{\Sigma F}{m} \\ &= -G\frac{M}{r^3}\vec{r} + \frac{f}{m} \end{aligned} \tag{19}$$

Where G is the gravitational constant, M is Doofenshmirtz' mass, m is the spacecraft's mass, which we also need to update throughout the simulation as it uses more of its fuel. $\vec{r}$ is the spacecraft's positional vector relative to Doofenshmirtz, making r the total distance from it. As we know, f is the thrust force the rocket engine exerts per second.

When simulating our rocket launches, we need to define the rocket's initial position and velocity. We'll launch our rocket from the equator, with initial coordinates

$$\begin{aligned} x_0 &= R \\ y_0 &= 0 \end{aligned}$$

in the planet frame, where R is Doofenshmirtz' radius.

A planet's rotational velocity is defined as

$$\begin{aligned} v_{\text{rot}} &= R\omega \\ &= R\frac{2\pi}{T} \end{aligned} \tag{20}$$

Where ω is its angular velocity, and T is its rotational period. Our rocket is initially rotating along with our home planet, which means that as soon as it launches, it has an initial velocity relative to it caused by its rotation. We assume that Doofenshmirtz rotates along the z-axis, and the spacecraft's initial velocity will therefore be

$$\begin{aligned} v_{0,x} &= 0 \\ v_{0,y} &= v_{\text{rot}} \end{aligned}$$

We'll need to take this into consideration when calculating whether or not our spacecraft has reached the necessary escape velocity yet, which is defined as

$$v_{\text{esc}} = \sqrt{\frac{2GM}{r}} \tag{21}$$

We'll do this by subtracting its initial absolute velocity $v_0 = v_{0,y}$ before checking if its current velocity v_i has reached v_{esc} yet.

After gathering information about how the launch simulation relative to the planet went, we may want to do some adjustments to our rocket, before simulation another launch. Because it's more realistic, we want to simulate the launch in the sun's frame of reference this time. We'll also compare our launch results with those of our research team to check if the simulations run by our software are accurate. They have defined the solar system coordinate system in such a way that out home planet is currently situated at $y_{\text{D}} = 0$ relative to the sun. This gives us the spacecraft's initial positional coordinates in the sun frame

$$\begin{aligned} x_0 &= x_{\text{D}} + R \\ y_0 &= 0 \end{aligned}$$

Where x_{D} is Doofenshmirtz' x-coordinate relative to the sun, which thankfully is supplied to us by our research team. The spacecraft's initial velocity is now also affected by our home planet's orbital velocity v_{orbit} around the sun. Our research team is fortunately kind enough to supply us with this as well, and we therefore find that our spacecraft's initial velocity in this frame of reference is

$$\begin{aligned} v_{0,x} &= v_{\text{orbit},x} \\ v_{0,y} &= v_{\text{orbit},y} + v_{\text{rot}} \end{aligned}$$

Once again we'll need to take this into consideration when checking whether or not our spacecraft has reached escape velocity yet, by subtracting the absolute initial velocity v_0 before checking if the current velocity v_i has reached this point yet.

IV. RESULTS

We had to check if our software was reliable enough to calculate estimates of the gas particles' velocities within one of the small gas boxes. Our first test was to see if it would manage to calculate the probability of a gas particle residing within the intervals

$$\begin{aligned} -1\sigma \leq& x - \mu \leq 1\sigma \\ -2\sigma \leq& x - \mu \leq 2\sigma \\ -3\sigma \leq& x - \mu \leq 3\sigma \end{aligned}$$

when we chose the mean μ to be zero. Our software calculated the following probabilities:

$$\begin{aligned} \pm 1\sigma &: 68.3\% \\ \pm 2\sigma &: 95.8\% \\ \pm 3\sigma &: 99.7\% \end{aligned}$$

which is a good sign considering the expected values are 68%, 95% and 99.7%, as we know from Lecture Notes 1A [1]. When studying the difference between the Gaussian probability distribution of the one-dimensional velocity component v_x versus the Maxwell-Boltzmann probability distribution of the absolute velocity v, our software gathered values that let us plot the graphs shown in Figure 2.

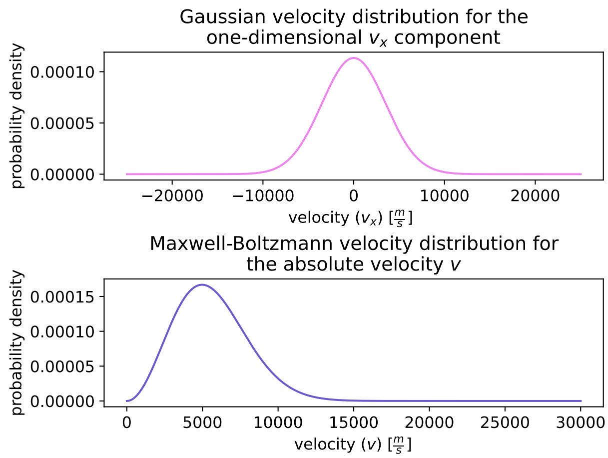


Figure 2. The Gaussian v_x-distribution (top graph) versus the Maxwell-Boltzmann absolute velocity distribution (bottom graph)

We calculated the probability of a particle's v_x-component existing within the interval

$$v_x \in [5 \times 10^3, 30 \times 10^3] \text{ m/s}$$

which we found to be approximately 7.76% of the particles. When there are a hundred thousand particles in the gas, this corresponds to about 7760 of them.

When simulating the energetic H_2 gas in a gas box within the rocket's combustion chamber, we found that the mean energy of the gas particles must be approximately

$$E_{\text{analytical}} = 6.21292 \times 10^{-20} \text{ J}$$

When the gas' temperature is 3000 Kelvins. We ran 5 simulations for one nanosecond each, and gathered the values displayed in Table I. Comparing these values, we found that the deviation between the maximum and minimum kinetic energies was approximately 39.15%.

Collisions	$E_{\text{numerical}}$	Error
777	5.00472×10^{-20}	19.45%
830	5.93310×10^{-20}	4.50%
761	5.13783×10^{-20}	17.30%
920	7.30773×10^{-20}	17.62%
829	6.03290×10^{-20}	2.90%

Table I. The amount of wall collisions for each of the 5 simulations with 100 particles, the approximated mean kinetic energy of a particle, and the relative error of this calculation when compared to the analytical result.

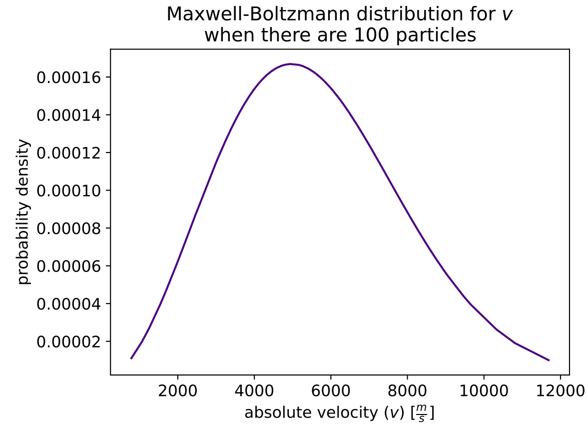


Figure 3. The absolute velocity distribution within one gas box when there are 100 particles in the box.

Figure 3 displays the Maxwell-Boltzmann distribution of the particles' absolute velocity v in a gas box from the last simulation where there were only a hundred gas particles in the box. When we increased the amount of particles to a hundred thousand, the absolute velocity distribution naturally became more realistic, as evident in Figure 4, which shows the results from the last simulation we did with this amount of particles.

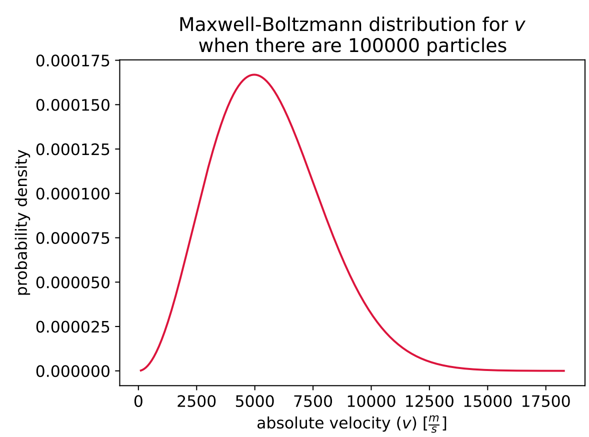


Figure 4. The absolute velocity distribution within one gas box when there are 100000 particles in the box.

Studying the distribution curve, we see that this fits well with the bottom graph in Figure 2, as the peak is at around $v = 5000$ m/s, and velocities above $v = 15000$ m/s are unrealistic. Comparing the values gathered from 5 simulations of this gas that are displayed in Table II, we found that the deviation between the maximum and the minimum kinetic energies calculated was approximately 0.62%.

Collisions	$E_{\text{numerical}}$	Error
837398	6.21275×10^{-20}	0.00%
838382	6.20191×10^{-20}	0.18%
838833	6.23043×10^{-20}	0.28%
836705	6.19176×10^{-20}	0.34%
838695	6.21829×10^{-20}	0.09%

Table II. The amount of wall collisions for each of the 5 simulations with 100 000 particles, the approximated mean kinetic energy of a particle, and the relative error of this calculation when compared to the analytical result.

After modelling a nozzle on each gas box, we found that the properties of one gas box with a hundred thousand gas particles within it at all times was

$$n = 3.5418 \times 10^{13}$$
$$f = 4.91288 \times 10^{-10} \text{ N}$$
$$m = 1.1856 \times 10^{-13} \text{ kg}$$

In one second, n is the amount of particles exiting the gas box, f is the average thrust force it exerts, and m is the amount of mass it loses. With this information in mind, we were able to calculate the corresponding properties for the entire combustion chamber, as we found that we'd need 1.6 $\times 10^{13}$ gas boxes to cover the entire bottom of the rocket and make up the chamber:

$$n = 2.8297 \times 10^{28}$$
$$f = 391078 \text{ N}$$
$$m = 94.7226 \text{ kg}$$

By using these parameters, we found through simulations that our rocket would use approximately 9954.4 kg fuel to boost its speed by $\Delta v = 1000$ m/s.

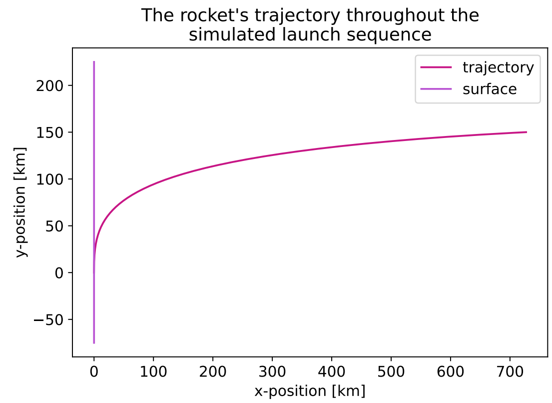
From these properties that we unveiled about our rocket's engine, we decided to initially try simulating a rocket launch from the planet's frame of reference, with 40000 kg fuel in our spacecraft's tank. To do this, we first had to calculate its initial velocity, which in this frame was simply our home planet's rotational velocity of approximately -372.47 m/s.

The spacecraft reached its escape velocity of approximately 10475 m/s after 7 minutes, and its positional coordinates relative to the launch site, as well as its velocity component relative to Doofenshmirtz are displayed in Table III.

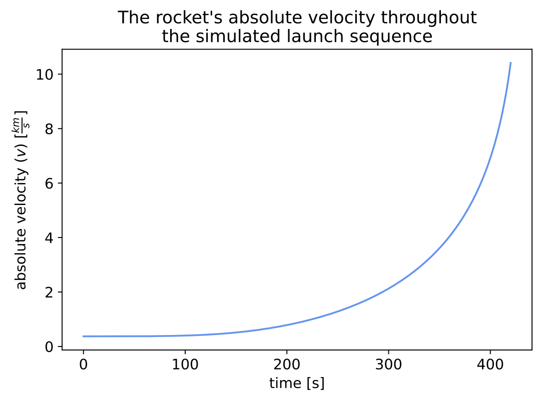
x [km]	y [km]	v_x [m/s]	v_y [m/s]
730.76	150.36	10508.80	329.35

Table III. Our spacecraft's positional coordinates relative to the launch site when reaching escape velocity, and its velocity components relative to the planet.

The spacecraft's trajectory during the launch is plotted along with the surface in Figure 5a, while its absolute velocity relative to the planet is shown in Figure 5b.



(a) Trajectory



(b) Velocity

Figure 5. The spacecraft's trajectory and velocity during the simulated launch from Doofenshmirtz' frame of reference.

Our rocket was left with 153.3 kg fuel after reaching escape velocity, which means that it used up 39846.8 kg of its fuel during the launch. We deemed this as too much when considering the journey we have planned, so we chose to increase the amount of fuel to 45000 kg. We also increased the amount of gas particles that we let into one gas box at once from 5 million to 6 million in hopes of increasing the rocket's thrust force to compensate for the added mass.

When simulating the rocket launch with the new parameters, it reached the escape velocity after 385 seconds, which is approximately 6 and a half minutes. It then had 1301.9 kg fuel left, which means it lost a total of 43698.1 kg during the launch sequence. This time, we wished to calculate our spacecraft's position and velocity relative to the sun, so we had to add Doofenshmirtz' orbital velocity to our spacecraft's initial velocity. Our research team thankfully supplied us with Doofenshmirtz' current velocity relative to the sun, which make up its current orbital velocity:

$$v_x = 0.0 \text{ km/s}$$
$$v_y = 26.48 \text{ km/s}$$

To compare these launch results to the last simulation, we've displayed the positional coordinates and velocities in Table IV both relative to the launch site, or the planet for the velocities, and to the sun.

	Planet frame	Sun frame
x [km]	850.94	5.30×10^8
y [km]	10125.90	10125.90
v_x [m/s]	10126.36	10161.71
v_y [m/s]	- 642.12	25837.83

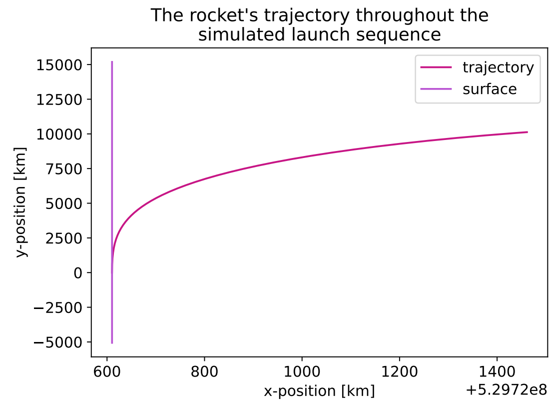
Table IV. Our spacecraft's positional coordinates relative to the launch site and to the sun when reaching escape velocity, and its velocity components relative to the planet and the sun.

Plots to help visualize the simulation in comparison to the last are shown in Figure 6.

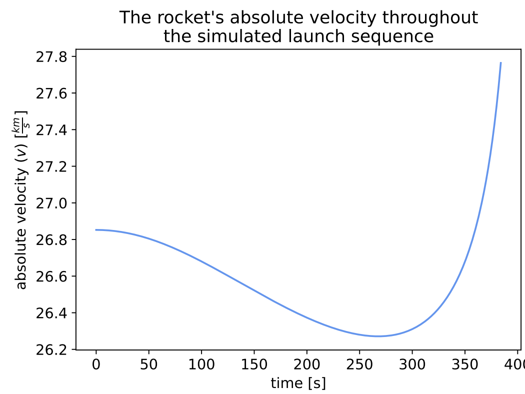
When comparing our simulated launch results to those gathered by our research team at the University of Oslo, we were pleased to hear that their simulation took 391.71 seconds, as our lasted for 385 seconds. However, our positional coordinates relative to the sun after we reached escape velocity in our simulation deviated with approximately

$$\Delta x \approx 136.13 \text{ km}$$
$$\Delta y \approx 373.35 \text{ km}$$

from our expected location, which was rather unfortunate.



(a) Trajectory



(b) Velocity

Figure 6. The spacecraft's trajectory and velocity during the simulated launch from the sun's frame of reference.

V. DISCUSSION

We saw that when testing our software, some of the calculated probability values deviated a little from what they were expected to be, namely the probability of a gas particle residing within the intervals

$$-1\sigma \leq v_x - \mu \leq 1\sigma$$
$$-2\sigma \leq v_x - \mu \leq 2\sigma$$

which we found to be

$$\pm 1\sigma : 68.3\%$$
$$\pm 2\sigma : 95.8\%$$

while we expected 68% and 95%. These deviations are small, but they still indicate minor flaws in our software. This may very well have played a role when simulating the energetic gas within the boxes that make up the rocket's combustion chamber, which could be the reason for the deviations in the calculated kinetic energies. In addition, simulations are always prone to round-off errors, especially when dealing with as small numbers as we are. This most likely also affected our results, both when simulating the gases and the launches themselves.

We wished to study the Gaussian probability distribution of the gas particles' v_x-component versus the Maxwell-Boltzmann probability distribution of their absolute velocity v. We noticed that the curve in the upper plot in Figure 2 is symmetrical, as expected of a Gaussian probability distribution. This tells us that for every particle with a velocity component v_x, there is another another particle in the gas with velocity $-v_x$. The mean velocity of the particles are $\mu = 0$ m/s, and therefore the graph has its peak at $v_x = 0$ m/s. Since all the particles have v_x, v_y and v_z-components, this does not necessarily mean that the mean absolute velocity is 0 m/s. This value, which is always a positive quantity, is defined as $v = v_x^2 + v_y^2 + v_z^2$. Thus, the second plot is not in conflict with the first, even though the curve is asymmetrical and has its peak at around 5000 m/s.

Not surprisingly, we found that the energy we calculated for the simulated gas deviated around 100 times more from the analytically calculated energy when there was only 100 particles in the gas, than when there were 100 000. Obviously, only a hundred gas particles in an energetic gas enclosed within such a gas box is very unrealistic, which we believe is why the results differ so much from each simulation (see Table I). However, when there are 100 000 particles in the gas, we still see that some of the simulations' relative errors are much larger than others (see Table II). As mentioned in the beginning of this section, basic round-off errors play a role in this, but approximating the gas as ideal when simulating it is also unrealistic. Particles collide with each other, and no collisions are completely elastic. These are also assumptions that we make when calculating the gas' total kinetic energy analytically however, so this shouldn't really affect our results.

During the launch simulations, we see that the spacecraft travels about the same distance in the x- and y-directions in both of them when looking at the coordinates relative to the launch site (see Tables 5 and 6). We believe that the small differences are mostly due to us changing the amount of fuel we brought, as well as the amount of particles in each gas box, which again increased the thrust force and fuel loss rate. However, when comparing Figures 5 and 6, we see that that the spacecraft's absolute velocity increases as expected in the planet frame. The spacecraft starts out with almost no velocity with respect to Doofenshmirtz, only the initial velocity caused by its rotation, which is minuscule when compared to the velocities it reaches as it gets further away from the planet and the gravitational pull becomes weaker. In the sun's frame of reference however, the curve looks different. We believe that the reason for this is that Doofenshmirtz' orbital velocity is added to its initial velocity when switching to the sun frame. As the spacecraft initially orbits around the sun along with Doofenshmirtz, its orbital velocity will decrease the further it moves away from the surface, since the gravitational pull becomes weaker. However, as it gets even further away from the planet, it keeps accelerating in the x-direction. This increase adds more to the absolute velocity than the gradual loss of orbital velocity, hence the slope at the end of the curve.

After the first launch simulation, we quickly noticed how little fuel we were left with. We tried running the simulation a couple more times with different parameters in hopes of reducing the amount of fuel used during the launch without it affecting the spacecraft's thrust force too much. What we landed on was the best we could seem to fix, but being left with only 1301.9 kg fuel, when the launch drained it of 43698.1 kg, doesn't sound too promising to us. After all, we are eventually going to travel through our solar system and visit another planet. We are unsure of what could be the reason for the extreme fuel loss and low thrust force in comparison, but we hope and believe it may have something to do with our simulation software.

When checking if our simulated launch results were reasonable compared to those that our research team calculated for us, we were disappointed to see that our spacecraft's final position deviated too much from where it should be. Figure 7 shows our rocket's simulated trajectory along with the position where we should have reached escape velocity according to our research team. As evident from the spacecraft's trajectory, we reach

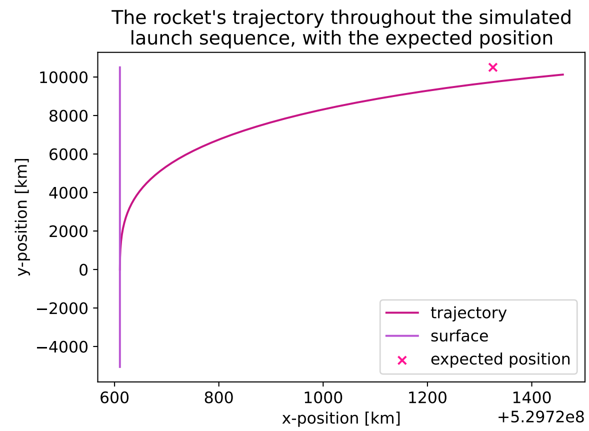


Figure 7. The spacecraft's trajectory during the simulated launch from the sun's frame of reference, with the correct position marked by the cross.

escape velocity further away from the surface than expected. This may be because of miscalculations in our simulation or round-off errors, but we also hypothesize that it could have something to do with our software not working completely as it should. There could possibly be a connection between the rocket's large fuel consumption and seemingly low thrust force, and the fact that we need to travel further and use more fuel to reach escape velocity. If the thrust force that our research team has calculated is larger than the one we calculated for our simulations, it would make sense for it to reach escape velocity closer to the surface. However, their simulation did take longer than ours, which again weakens this hypothesis.

VI. CONCLUSION

We learned a lot about statistical physics, specifically the Gaussian and Maxwell-Boltzmann probability distributions, and we were able to use these to simulate the conditions within our rocket's combustion chamber. This made it possible for us to determine parameters for its engine, and use this to simulate rocket launches. We did this both with respect to our home planet Doofenshmirtz and with respect to the sun, and compared the results from the latter simulation to that of our research team. We were unsuccessful in correctly calculating its position as it reaches the escape velocity, but our simulations took approximately the same amount of time, and it seemed like we weren't too far off.

For whatever mysterious reason, our rocket engine burns through enormous amounts of fuel when trying to accelerate and launch from our planet, which may lead to troubles later when we eventually will perform an actual launch and travel to a destination far away. Thankfully, our research team promised us that they would take a look at our simulation software as well as our rocket's engine to hopefully be able to help us figure out some kind of a solution to this issue.

REFERENCES

[1] Hansen F. K. *Lecture Notes 1A*. URL: https://www.uio.no/studier/emner/matnat/astro/AST2000/h22/undervisningsmateriell/lecture_notes/part1a.pdf.

Appendix A: Deriving an expression for FWHM

We have

$$f(\mu,\sigma,x) = \frac{1}{\sqrt{2\pi}\sigma}\exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \tag{A1}$$

And we know that the maximum of this function is when $x=\mu$, where μ is the mean value. This gives us

$$f_{\text{max}} = f(\mu) = \frac{1}{\sqrt{2\pi}\sigma} \tag{A2}$$

The function value at half maximum is therefore

$$f_{\text{halfmax}} = f(\mu) = \frac{1}{2\sqrt{2\pi}\sigma} \tag{A3}$$

We can use this to determine what x needs to be to get $f(x) = f_{\text{halfmax}}$, as the half maximum is achieved when

$$\exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] = \frac{1}{2} \tag{A4}$$

We get

$$\begin{aligned}
-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2 &= \ln\left(\frac{1}{2}\right)\\
\left(\frac{x-\mu}{\sigma}\right)^2 &= -2\ln\left(2^{-1}\right)\\
\frac{x-\mu}{\sigma} &= \pm\sqrt{2\ln 2}\\
x-\mu &= \pm\sqrt{2\ln 2}\sigma
\end{aligned} \tag{A5}$$

Since the Gaussian probability distribution is symmetric, we know that the width $|x-\mu|$ is equal for each of the x-values that grant us $f(x) = f_{\text{halfmax}}$. By the definition of the Full Width at Half Maximum we therefore get

$$\begin{aligned}
\text{FWHM} &= 2|x-\mu|\\
&= 2\sqrt{2\ln 2}\sigma \quad \square
\end{aligned} \tag{A6}$$

We can of course use this to express the standard deviation σ in the following way:

$$\sigma = \frac{\text{FWHM}}{\sqrt{8\ln 2}} \tag{A7}$$

Appendix B: The mean velocity of a gas particle

From the Maxwell-Boltzmann probability distribution we have

$$P(v)dv = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}} 4\pi v^2 dv \tag{B1}$$

By integrating the expression $vP(v)dv$ from 0 to ∞, we can find an expression for the mean absolute velocity $\langle v \rangle$ of a gas particle:

$$\begin{aligned}
\langle v \rangle &= \int_0^\infty v \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}} 4\pi v^2 dv \\
&= \left(\frac{m}{2\pi kT}\right)^{1/2} \int_0^\infty 4\pi v^3 \frac{m}{2\pi kT} e^{-\frac{1}{2}\frac{mv^2}{kT}} dv \\
&= \left(\frac{m}{2\pi kT}\right)^{1/2} \int_0^\infty 4v \frac{mv^2}{2\pi kT} e^{-\frac{1}{2}\frac{mv^2}{kT}} dv
\end{aligned} \tag{B2}$$

We make the following substitution:

$$u = \frac{1}{2}\frac{mv^2}{kT} \tag{B3}$$

which gives us

$$dv = \frac{kT}{mv} du \tag{B4}$$

We then add this to (B2):

$$\begin{aligned}
\langle v \rangle &= 4\left(\frac{m}{2}\right)^{1/2} \int_0^\infty vue^{-u} \frac{kT}{mv} du \\
&= \frac{4kT}{m} \left(\frac{m}{2\pi kT}\right)^{1/2} \int_0^\infty ue^{-u} du \\
&= \left(\frac{16k^2T^2}{m^2} \frac{m}{2\pi kT}\right)^{1/2} \\
&= \sqrt{\frac{8kT}{m\pi}} \ \square
\end{aligned} \tag{B5}$$

Appendix C: Proving the ideal gas law

We know from Lecture Notes 1A [1] that the Maxwell-Boltzmann distribution for momentum $p = mv$ is defined as

$$P(p)dp = \left(\frac{1}{2\pi mkT}\right)^{3/2} e^{-\frac{1}{2}\frac{p^2}{mkT}} 4\pi p^2 dp \tag{C1}$$

By combining this with what is defined as the *pressure integral*, we can derive the ideal gas law:

$$\begin{aligned}
P &= \frac{1}{3}\int_0^\infty pvn(p)dp \\
&= \frac{1}{3}\int_0^\infty p\frac{p}{m} nP(p)dp \\
&= \frac{n}{3m}\int_0^\infty p^2 \left(\frac{1}{2\pi mkT}\right)^{3/2} e^{-\frac{1}{2}\frac{p^2}{mkT}} 4\pi p^2 dp
\end{aligned} \tag{C2}$$

We make the following substitution:

$$u = \frac{1}{2}\frac{p^2}{mkT} \tag{C3}$$

which gives us

$$dp = \frac{mkT}{p} du \tag{C4}$$

We apply this to (C1) and get

$$\begin{aligned}
P &= \frac{n}{3m}\int_0^\infty p^2 \left(\frac{1}{2\pi mkT}\right)^{3/2} e^{-u} 4\pi p^2 \frac{mkT}{p} du \\
&= \frac{n}{3m}\frac{4}{\sqrt{\pi}}\int_0^\infty p^3 \left(\frac{1}{2mkT}\right)^{3/2} e^{-u} mkT du \\
&= \frac{n}{3}\frac{4}{\sqrt{\pi}} kT \int_0^\infty \left(\frac{p^2}{2mkT}\right)^{3/2} e^{-u} du \\
&= \frac{n}{3}\frac{4}{\sqrt{\pi}} kT \int_0^\infty \left(u^{3/2}\right)^{3/2} e^{-u} du \\
&= \frac{n}{3}\frac{4}{\sqrt{\pi}} kT \frac{3}{4}\sqrt{\pi} \\
&= nkT \ \square
\end{aligned} \tag{C5}$$

Appendix D: The mean energy of a gas particle

We have the following expression for an object's kinetic energy:

$$E_K = \frac{1}{2}mv^2 \tag{D1}$$

Since ideal gases don't have intermolecular forces, we can use the Maxwell-Boltzmann probability distribution again to calculate the mean energy of a gas particle by integrating the expression $E_K P(v)dv$ from 0 to ∞:

$$\begin{aligned}\langle E\rangle &= \int_0^\infty E_K P(v)dv \\ &= \int_0^\infty \frac{1}{2}mv^2 \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}} 4\pi v^2 dv \\ &= \frac{2\pi m}{\pi^{3/2}} \int_0^\infty v^4 \left(\frac{m}{2kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}} dv \\ &= \frac{2m}{\sqrt{\pi}} \int_0^\infty v \left(\frac{mv^2}{2kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}} dv\end{aligned} \tag{D2}$$

We once again make the substitution

$$u = \frac{1}{2}\frac{mv^2}{kT} \tag{D3}$$

and get

$$dv = \frac{kT}{mv}du \tag{D4}$$

Which we then add to (D2):

$$\begin{aligned} &= \frac{2m}{\sqrt{\pi}} \int_0^\infty v u^{3/2} e^{-u} \frac{kT}{mv} du \\ &= \frac{2kT}{\sqrt{\pi}} \int_0^\infty u^{3/2} e^{-u} du \\ &= \frac{2kT}{\sqrt{\pi}} \frac{3\sqrt{\pi}}{4} \\ &= \frac{3}{2}kT \ \square \end{aligned} \tag{D5}$$