AST2000 Lecture Notes

Part 1A Statistics and gas dynamics: building the rocket engine

Questions to read before the lecture

- 1. What does the normal distribution (also called the Gauss distribution) look like? (can you make a rough drawing?)
- 2. Can you think of an example of something which is random?
- 3. What is a statistical distribution function?
- 4. What is an ideal gas?
- 5. If you have hydrogen gas at the temperature T=6000K. With what velocity do the particles move?
- 6. What makes a rocket accelerate?



Testing a rocket engine. (Photo:SpaceX)

AST2000 Lecture Notes

Part 1A

Statistics and gas dynamics: building the rocket engine

1 Gaussian statistics

In this section we will give a very basic and nonrigorous introduction to some statistical concepts which we will use during the course. Given a random variable x, the probability distribution P(x)gives the probability that x will have a given value. When normalized, the probability runs from P(x) = 0 for a value which can never occur to P(x) = 1 for a value which occurs with 100% probability.

You might wonder what statistics has to do with the construction of a rocket engine, the main goal of this section. In order to calculate the thrust of a rocket engine, we need to simulate the gas particles which escape the nozzle. To simulate gas particles, we need to know their velocities. These are random, and as we will see, Gaussian distributed. We therefore need statistics in order to find the initial conditions of the gas particles. But there will also be several other uses of statistics during this course.

To make it easier and more intuitive, we will use an example from everyday life: the distribution of heights of women. The distribution of human height follows roughly what is called the *normal* distribution or the Gauss distribution. It can be written as

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

where μ is what we call the mean value and σ is the standard deviation. The standard deviamean value.

Note that P(h) is a probability density. If you look at the units, you can see that it is m^{-1} . In order to get a probability, you need to multiply with a tiny height interval Δh . In fact, the interval should be so small that we write it as in infinitesimal dh. You can therefore use P(h)dh to find the probability of a woman to have a height in the range between [h, h + dh] where dh is a very small height interval. We will now see how to use the distribution in practice for larger intervals.

Using the Gaussian distribution

Norwegian women have a mean height of about $\mu = 168$ cm with a standard deviation of roughly $\sigma = 6$ cm. In figure 1 we show this distribution (note that the real distribution deviates slightly from the Gaussian which we have plotted here). The distribution, being symmetric, is centered on the mean value with a width which depends on the standard deviation as shown in the plot.

The probability for a woman to have a height between h_1 and h_2 is given by

$$P(h_1, h_2) = \int_{h_1}^{h_2} P(h)dh$$

Now, before you continue to read, try to find out (without doing the integral) what would be the results of this integral with $h_1 = 0$ and $h_2 = \infty$?

Did you find a value? Let's rephrase the question: what is the probability for a woman to have tion shows what is a common deviation from the a height between 0 and infinity? It is of course 100% which means a probability of 1. The Gaussian probability is normalized to 1 for an integral going from $h=-\infty$ to $h=+\infty$. Here you see one of the reasons why heights do not follow a completely Gaussian distribution: Negative heights do not make sense, also very low or high positive heights are meaningless while the Gaussian distribution is valid for all values of h. As the probability drops very quickly towards zero and for very large heights, this is not a problem in practice. Although the integral is performed starting at h=0 instead of $h=-\infty$, the results will still be very close to 1.

In order to get a feeling for the meaning of σ , in the exercises you will calculate the probability for a woman to have

- a height between $\mu \sigma$ and $\mu + \sigma$
- a height between $\mu 2\sigma$ and $\mu + 2\sigma$
- a height between $\mu 3\sigma$ and $\mu + 3\sigma$

The answers you will find are 68%, 95% and 99.7% respectively. We have already seen that σ defines the width of the distribution. Now we see exactly what it means: 68% of the area under the curve is found between $\mu - \sigma$ and $\mu + \sigma$ as shown in the figure. A large standard deviation thus means that the curve is wide and that it is common to find values far away from the mean value. On the contrary, a small standard deviation gives a very sharp curve and values which are normally very close to the mean.

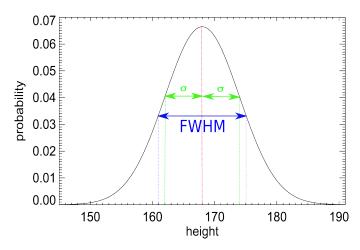


Figure 1: The Gaussian probability distribution, here as an approximation to the probability distribution for the heights of Norwegian women.

A more intuitive measure for the width of the distribution is given by FWHM, Full Width at Half Maximum. It is a measure of the width of the curve at half its maximum value as shown in the figure. In the exercises you will show that the relation between the standard deviation and the FWHM is given by

$$\sigma = \frac{\text{FWHM}}{\sqrt{8 \ln 2}}.$$
 (2)

We are now ready to answer the following question: How many women in Norway are taller than 190cm? First we need to calculate the probability for a woman to be taller than 190cm, thus the probability for a woman to have a height between 190cm and infinity:

$$P = \int_{190}^{\infty} P(h)dh$$

Doing the integral numerically we find 0.01%. Having the probability, we need the number of women: there are roughly 2 million adult women in Norway in 2016, so this gives a total of about 246 women taller than 190cm.

1.2 Redefining mean and standard deviation

Assume you have a set of *sample values*, random numbers drawn from a given distribution. Let's use our example above: say you have the heights x_i of N=1000 women i=[1,1000]). In this case we are used to calculate the mean value as

$$\langle x \rangle = \frac{1}{N} \sum_{i=1}^{N} x_i \tag{3}$$

Note that we use $\langle \rangle$ to denote the mean value. Similarly, the standard deviation is the expected deviation from the mean. The deviation of x_i from the mean is $(x_i - \langle x \rangle)$. The standard deviation should therefore be the mean value of this. But clearly this is zero as the deviation will sometimes be positive and sometimes negative. What we want is the absolute value of the deviation. The square of the standard deviation is therefore defined as $\langle (x - \langle x \rangle)^2 \rangle$:

$$\langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{N} \sum_{i=1}^N x_i^2 - \left(\frac{1}{N} \sum_{i=1}^N x_i\right)^2$$

(did you understand what was happening here? If not, try to substitue $\langle \rangle$ with $\frac{1}{N} \sum_i$ and see if you can arrive at the expression on the right hand side.) For a Gaussian distribution, these two expressions (for the mean and standard deviation) converge to μ and σ^2 when the number of samples N is sufficiently large. Note that there should really be N-1 in the denominator instead of N, but in most applications in physics and astrophysics, N is so large that we can assume $N \approx N-1$.

It can be shown that one can also find the mean value from a given distribution P(x) by taking its first moment:

$$\mu = \langle x \rangle = \int_{-\infty}^{\infty} x P(x) dx$$
 (4)

This expression is not really needed for the Gaussian distribution where the value of the mean value μ is evident from the expression for the distribution. We will see later in this course however that it can be very useful for other distributions where the mean value is not known.

Thinking about it, these two expressions for the mean (eq. 3 and 4) are the same in the limit $N \to \infty$. In the latter expression you take the weighted mean of all possible values of heights, giving a high weight to the more probable values and a low weight to the less probable values. In the former expression, the more probable numbers will occur much more often in the sum than the less probable numbers, giving in a similar manner more weight to the more probable values.

Similarly the standard deviation from a distribution can be found from the second moment:

$$\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \int_{-\infty}^{\infty} x^2 P(x) dx - \mu^2$$

Finally, you can also find the mean value of a function of your random variable, f(x),

$$\langle f(x) \rangle = \frac{1}{N} \sum_{i=1}^{N} f(x_i)$$

by

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)P(x)dx$$

As an example of the latter expression, let us use the Body Mass Index (BMI) which is defined as

$$BMI = \frac{m}{h^2}$$

where m is the mass (weight) of the person and h is the height. Say we want to find the mean BMI of all women with a given mass $m=70\mathrm{kg}$. Then we have

$$\langle BMI \rangle = \int_0^\infty \frac{70 \text{kg}}{h^2} P_h(h) dh$$

Note again that the integral for the mean (following the equation above) is supposed to start at $h = -\infty$, but as negative heights do not make sense, we start at h = 0.

In the exercises you will test these expressions for the Gaussian distribution.

1.3 Multidimensional distributions

We have been using the distribution of heights $P_h(h)$ as an example. We will now ask the question: What is the probability for a woman to have a height between h = [170cm, 175cm], an IQ between IQ = [120, 130] and a (diastolic) blood pressure between p = [70, 79]mm Hg. Thus we are looking for the probability for all these conditions to be fulfilled simultaneously.

IQ in the population is Gaussian distributed with mean IQ = 100 and standard devition 16. The distribution of diastolic blood pressure (the lowest of the two numbers used to denote blood pressure) is roughly Gaussian distributed with mean value about $p=80 \mathrm{mm}$ and standard deviation about 10mm for a healthy person.

In order to answer the above question, we need to know that probabilities are multiplicative: If the body height, IQ and blood pressure are unrelated (which is probably not completely correct, but we will make this assumption here), then the joint probability distribution for all these 3 measures is simply given as

$$P(h, IQ, p) = P_h(h)P_{IQ}(IQ)P_p(p)$$
 (5)

It is easy to convince yourself that this makes sense: Assume you want to know the probability for a woman to have a height which is average or lower, a blood pressure which is average or lower and which may have any IQ. The probability to have a height or blood pressure lower than average is 0.5. The probability to have any IQ is 1. Thus, the total probability is $P = 0.5 \times 0.5 \times 1 = 0.25$ which equals 1/4. This makes sense: out of 4 women, on average 2 (50%) will have a height below the mean. Of these two, on average one (50%) will have a blood pressure below average. Thus one of the four satisfy our condition.

Now we are ready to solve the question starting this subsection. The answer must be given by

$$P = \int_{170}^{175} dh \int_{120}^{130} dIQ \int_{70}^{79} dp \, P_h(h) P_{IQ}(IQ) P_p(p) \, \mathbf{2}$$

1.4 The central limit theorem

Why is the Gaussian or normal distribution called 'normal'? Why are we focusing on this distribution here? Why is it so important? One of the main reasons for this comes from the *central limit theorem*.

Assume that you have M sets of N independent random numbers $x_1, x_2, ..., x_N$ drawn from **any** probability distribution (the distribution needs to be the same for all N samples in all M sets). For each of the M sets, form the average a_j (j = [1, M]) of the N numbers in the given set. Then the central limit theorem states that given some conditions on the distribution and that N is sufficiently large, the probability distribution of a_j will be approximately Gaussian. Given some further conditions, the theorem holds even if the numbers $x_1, x_2, ..., x_N$ are drawn from different distributions. We will not study the details of the necessary conditions for the central limit theorem to hold in this course.

The result is that observables in nature that originate from complicated processes with complicated probability distributions will often have a nearly Gaussian distribution as most measurements involves taking the mean over numbers in some form. Take for instance the measurement of blood pressure: the measurement pro-

cess takes some finite time Δt . During this time, the blood pressure has already been fluctuating randomly with some unknown and possibly complicated probability distribution. The measurement you get is the mean over these fluctuations and the central limit theorem may therefore apply when you make statistics based on several measurements of the blood pressure giving close to a normal distribution.

This is a simplified explanation for why we often find Gaussian distributions when studying very different phenomena from the human body, to weather statistics and even the velocity of particles in a gas.

Before proceeding to the next section, you should do exercise 1A.1 - 1A.3.

2 Velocities of particles in a gas: Maxwell-Boltzmann

Now we are ready to see how Gaussian statistics can be used to reach our goal. First we will look at the velocity components of the gas particles, then we will look at the absolute velocity.

In this course we will mostly be using the *ideal* gas approximation. In the ideal gas approximation, the gas particles are assumed not to have any extension (they are point like) and they do not interact with each other except that they collide elastically. Elastic collisions mean that their kinetic energy is conserved in the collision. As long as the temperature and pressure in a gas are not extremely high or low, most gases can, with a very good approximation, be treated as ideal gases.

2.1 Velocity components of gas particles

The velocity $\vec{v} = (v_x, v_y, v_z)$ of particles in an ideal gas is random following a Maxwell-Boltzmann probability distribution. You will deduce this distribution later in courses on statistical mechanics. However, since it is impossible to do astrophysics without some basic knowledge of the laws of thermodynamics and statistical physics, we will anticipate some of the results from later courses already. The Maxwell-Boltzmann distribution can be written as

$$P(\vec{v}) = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}},$$

(here k is Boltmann's constant) giving the probability that a gas particle with mass m in a gas with temperature T has the velocity vector \vec{v} . This is the vector form of the Maxwell Boltzmann distribution. It might not be directly evident that this is a Gaussian distribution. We therefore rewrite this as

$$P(\vec{v}) = \frac{1}{(2\pi\sigma^2)^{3/2}} e^{-(v_x^2 + v_y^2 + v_z^2)/(2\sigma^2)}$$

with $\sigma = \sqrt{kT/m}$. Before reading on, check that the two equations are indeed identical.

We further write this as

$$\begin{split} P(\vec{v}) &= \\ &\frac{1}{\sqrt{2\pi}\sigma} e^{-v_x^2/(2\sigma^2)} \times \frac{1}{\sqrt{2\pi}\sigma} e^{-v_y^2/(2\sigma^2)} \times \frac{1}{\sqrt{2\pi}\sigma} e^{-v_z^2/(2\sigma^2)} \\ &= P(v_x) P(v_y) P(v_z). \end{split}$$

This is a product of three independent Gaussian distribution functions. Compare with equation 5. We see that the distribution of velocities v_x , v_y and v_z in each dimension x,y and z are independent of each other and Gaussian with mean value $\mu = 0$ and standard deviation $\sigma = \sqrt{kT/m}$. This makes sense: if we take the x-direction as an example, it is easy to understand that the mean value of v_x must be zero, the probability for a random gas particle to have a positive or negative velocity in the x-direction is equal. It also makes sense that the distribution is equal in all three dimensions (they all have the same σ): there is no reason that the velocities in one dimension should be different from the other dimensions. It also makes sense that the velocities in the three dimensions are independent: there is no reason why the velocity in the x-direction should influence the velocity in the y-direction.

We can therefore conclude that in order to simulate gas particles with a given mass m and gas temperature T, we need to draw independent random Gaussian numbers for each dimension x, y and z in order to find initial particle velocities. In python you can draw a random number from a Gaussian distribution function using

number=random.gauss(mean,sigma)

(note that you first need import random) The numbers are drawn from a random number generator which is not completely random, but draws pseudo-random numbers which are very close to having the specified Gaussian distribution. Note that the random number generator should be given an initial seed value by

random.seed(seed_value)

where the seed value is a value which can be any integer. This should be done only once in the beginning of the code. This ensures that the sequence of random numbers which is generated will always be the same every time you run the code. If you want to run the code with a different sequence of random numbers you must change the seed value. You should always do this when the code is working, in order to check that the results do not depend strongly on a given sequence of random numbers.

In exercise 1A.6 you will draw random gas particle velocities in python in order to simulate the gas in the rocket engine.

2.2 The absolute velocity of gas particles

We have so far looked at the velocity components of the gas particles and found that these are independent and Gaussian distributed. For several applications, we are more interested in the absolute value of the particle velocities rather than the components. We would like to find the probability distribution P(v) rather than $P(\vec{v})$. Later in this course you will learn how to deduce the former from the latter, for now we will only state the result. This is the form of the Maxwell-Boltzmann distribution which we will use most during this course. For an ideal gas at temperature T (measured in Kelvin K), the fraction of particles in the gas in a given velocity range [v, v + dv] is given by the

Maxwell-Boltzmann distribution function

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

where m is the mass of the atoms in the gas.

The meaning of the function is the following: if you insert the temperature T as well as the mass m of the particles in the gas you can find the fraction of particles which have a velocity in the range [v, v + dv] (or, the probability that a particle has a velocity in the range [v, v + dv]). Here dv is a tiny velocity interval. If you want to find the number of particles per volume (number density) with the given velocity, you simply multiply with the total number density:

$$n(v)dv = nP(v)dv (6)$$

where n is the total number of particles per volume of the gas and n(v)dv is defined the total number of particles per volume with a velocity in the range [v, v + dv]. Say you need to find out how many atoms have the velocity in the range between 2 and 2.01 km/s. Then you insert v=2 km/s to obtain n(v), and use $dv=\Delta v=0.01$ km/s and use n(v)dv to find the total number of atoms with the given velocity per volume.

Note again the notation: we use P(v) for the probability distribution meaning the probability that a particle has a certain velocity (or the fraction of particles with this velocity) while n(v) is the number density of particles with this velocity. The difference between the two is only the normalization: integrating over all values of v, the probability integrates to 1 while the density integrates to the total number density n. Also remember from above that both P(v) and n(v) need to be multiplied with (or integrated over) a tiny velocity interval dv in order to give a meaningful number.

In figure 2 we see two such distributions, both for hydrogen gas (the mass m has been set equal to the mass of the hydrogen atom), solid line for temperature T=6000 K which is the temperature of the solar surface and dashed line for T=373 K (which equals 100 °C). We can thus use this distribution to find the percentage of molecules in a gas which has a certain velocity. Now, before you read on, go back and make sure

that you understand well the meaning of the function P(v) and n(v).

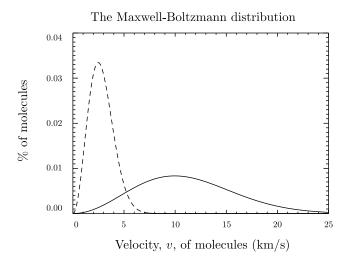


Figure 2: The Maxwell-Boltzmann distribution for hydrogen gas, showing the percentage of molecules in the gas having a certain thermal velocity at temperature T = 6000 K (solid line) and T = 373 K (dashed line).

Like $P(\vec{v})$, also P(v) is a probability distribution function for velocity. We already saw that $P(\vec{v})$ is a Gaussian distribution with mean value 0. Clearly P(v) cannot have a mean value of zero as v=0 is the lowest possible absolute velocity. The question now is, (1) what is the mean value of the absolute velocity in a gas? and (2) is P(v) also a Gaussian distribution? Try first to answer question (2). Look at the expression and make up your mind before proceeding.

Looking at the expression for P(v) we see that there is also some v dependence outside the exponential which cannot occur for a Gaussian distribution. P(v) is therefore not Gaussian. How then, can we find the mean absolute velocity of particles in a gas? Look back to the section on Gaussian statistics and see if you can find the solution.

Did you find out how to do it? Here is the answer: We learned that in order to find the mean value from a given distribution, one has to use equation 4. Here we go:

$$\langle v \rangle = \int_0^\infty v P(v) dv \tag{7}$$

$$= \int_0^\infty v \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-\frac{1}{2}\frac{mv^2}{kT}} 4\pi v^2 dv.$$
 (8)

In exercise 1A.5 you will solve the integral and momentum before the collision. This means simfind the expression for the mean velocity.

3 The pressure of a gas

Before we can simulate our rocket engine, we need to learn a few more thermodynamic concepts which we also will need on several other occasions during this course. The first one is pressure. We will now define pressure and deduce an analytical expression for the pressure in a gas. Then we will measure the pressure numerically in a gas of simulated particles. This will be the first step towards our rocket engine simulation.

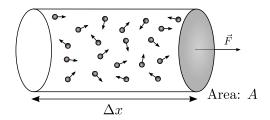


Figure 3: Pressure on the wall of area A is the total force exerted from the particles within the cylinder divided by the area.

To calculate the pressure of a gas we need to consider the force that particles in a gas exert on a wall (real or imaginary). Pressure is defined as the force per area on the wall P = F/A from the particles in the gas. In figure 3 we see particles within a cylinder of length Δx . The particles collide with the wall at the right end of the cylinder. The surface area of the part of the wall limiting the cylinder on the right end is A. We will assume that the collisions are elastic. We remember that in elastic collisions the kinetic energy of the particle is conserved. For this to be the case in the collision with the wall, the total absolute value of the momentum of the particle is conserved (can you see this?). If we define the x-direction as the direction towards the wall and the y-direction as the direction along the wall (see again figure 3), then momentum p_y in y-direction is always conserved since there is no force working in that direction. For the absolute value of the momentum to be conserved, the absolute value of the momentum p_x in the x-direction must be conserved. This means that the momentum in the x-direction after the collision must the $-p_x$ where p_x is the ply that the incoming angle equals the outgoing angle (see figure 4).

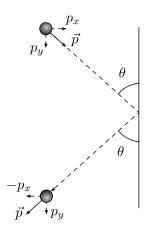


Figure 4: An elastic collision: the absolute value of the momentum is conserved.

Before the collision, a particle has momentum (p_x, p_y) . After the collision the particle has momentum $(-p_x, p_y)$. The total change in momentum is just $2p_x$. The force exerted on the wall during a time interval Δt is according to Newton's second law

$$f = \frac{dp}{dt} \approx \frac{\Delta p}{\Delta t} = \frac{2p_x}{\Delta t}.$$
 (9)

We will now consider a time interval Δt such that all the particles within the cylinder with velocity $|v_x|$ and momentum $|p_x|$ has collided with the wall within time Δt . The time it takes a particle with x-velocity v_x at a distance Δx from the wall to hit the wall is $\Delta t' = \Delta x/v_x$. Within the time $\Delta t'$, all the particles in the cylinder traveling in the direction towards the wall (with velocity v_x) have collided with the wall. But only half of the particles travel in the direction towards the wall. The other half travels in the opposite direction and had therefore already hit the wall within a time interval $\Delta t'$ earlier. So within the time

$$\Delta t = 2\Delta t' = \frac{2\Delta x}{v_x}$$

every single particle in the cylinder with velocity $|v_x|$ has collided with the wall. Inserting this in equation 9 we find that the force exerted by any single particle of velocity $|v_x|$ and momentum $|p_x|$ in the cylinder within the time Δt is

$$f = \frac{2p_x}{\Delta t} = \frac{v_x p_x}{\Delta x}.$$

The total velocity is given by $v^2 = v_x^2 + v_y^2 + v_z^2$, but on average the velocity components are equally distributed among all three dimensions such that the mean values $\langle v_x^2 \rangle = \langle v_y^2 \rangle = \langle v_z^2 \rangle$ giving that $v^2 = 3v_x^2$ or $v_x = v/\sqrt{3}$ (note: this will not be true for one single particle, but will be true when taking the average over many particles) on average. Exactly the same argument holds for the momentum giving $p_x = p/\sqrt{3}$. We thus have

$$p_x v_x = \frac{1}{3} p v.$$

such that

$$f = \frac{vp}{3\Delta x}.$$

We have already seen the Maxwell-Boltzmann distribution function for an ideal gas in the form of a number density n(v) (equation 6) which gives the number of gas particles with a certain velocity. There is also a Maxwell-Boltzmann distribution function for momentum, n(p), which gives us the number density of particles in an ideal gas with momentum p such that n(p)dp is the number of particles with momentum between p and p + dp. We will later deduce the shape of this distribution function. For now we will assume a general distribution function n(p). Since n(p) is a number density, i.e. number per unit volume, we can write the total particles in the cylinder N(p) with momentum p as the density times the volume $A\Delta x$ of the cylinder

$$N(p) = n(p)A\Delta x.$$

The total force exerted on the wall of the cylinder by particles of momentum p is then

$$dF = \frac{pv}{3\Delta x} N(p) dp = \frac{1}{3} p v n(p) A dp,$$

or in terms of the pressure exerted by these particles

$$dP = \frac{dF}{A} = \frac{1}{3} p v n(p) dp. \tag{10}$$

We obtain the total pressure by integrating

$$P = \frac{1}{3} \int_0^\infty p \, v \, n(p) \, dp \tag{11}$$

which is the pressure integral. Given the distribution function n(p) (for instance the Maxwell-Boltzmann distribution) and an expression relating v and momentum p (for instance v = p/m

for non-relativistic particles) we can integrate this equation to obtain the pressure in the gas.

In exercise 1A.6 you will simulate gas particles in a cube and measure the force that the gas particle exert on one of the walls in order to measure the pressure in the gas. In order to do that exercise you need to

- Given the length L of the sides of the cube, you need to generate the random positions of the N gas particles
- Generate the random velocities in each direction v_x , v_y and v_z for all N particles
- Follow the movement of the gas particles with time. Remember that the particles have constant velocity until they hit a wall.

You already now how to solve the second point here. We will now discuss the first point: The positions of the gas particles are random, but with which probability distribution? Is it also Gaussian? If so, what would be the mean and the standard deviation? Think about this before reading on.

Did you realize how the distribution must look like? Do you understand why it cannot be Gaussian? We will begin looking at the x position: If the gas is homogeneously distributed, it must be equally probable to find a gas particle at any point between x=0 and x=L. This is what we call a uniform probability distribution. The uniform distribution $P_{\text{uni}}(x)$ gives an equal probability for x to have any value within a certain range. In python you can draw a random number between x_1 and x_2 from a uniform distribution using

number=random.uniform(x1, x2).

4 The equation of state: the relation between temperature, pressure and density

We will now use the pressure integral above to deduce one of the most important laws of thermodynamics: the ideal gas law which is the equation of state (the relation between temperature, pressure and density) for an ideal gas. We see from equation 11 that in order to find an expression

for the pressure in a gas, we need the distribution function n(p) in terms of momentum. We already know the Maxwell-Boltzmann distribution function for velocity, but we need to rewrite in in terms of momentum. This is the expression we know:

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

It is important here to note the differential dv which also needs to be transformed. Let us assume non-relativistic gas such that p = mv. Then dv = dp/m. Inserting we thus get:

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

Further, remember that the number density distribution n(p) is simply the probability distribution multiplied by the total number density n(p) = nP(p). Inserting everything in the pressure integral and using p = mv, we have

$$P = \frac{n}{3} \int_0^\infty \frac{p^2}{m} \left(\frac{1}{2\pi mkT} \right)^{3/2} e^{-\frac{1}{2} \frac{p^2}{mkT}} 4\pi p^2 dp$$
 (12)

In the exercise 1A.5 you will show that this equals

$$P = nkT$$

which is the equation of state for an ideal gas. This relation will be used several times during this course. As an example of a practical application, one can easily see that this equation explains why the pressure in a gas increases when the temperature or density increase.

Before proceeding to the next section, you should do exercise 1A.4 - 1A.5.

5 Simulating gas particles: building a rocket engine

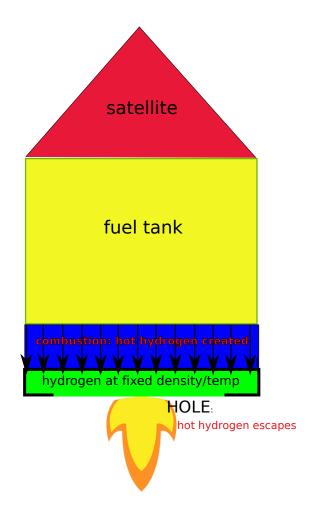


Figure 5: A simplified model of a rocket.

After a brief introduction to statistics and thermodynamics we are now ready to face our original problem. In section 3, we already discussed how to generate the random position and velocities of the gas particles in a box. If the gas density/temperature is high and we make a hole in the box on one side such that the particles can escape, we already have a rocket engine: particles with momentum escape in one direction and in order to conserve momentum the box has to move in the opposite direction.

In figure 5 we show a very simplified model of a rocket. On the top is our satellite, then below the fuel tank is the combustion chamber where the fuel is converted to hydrogen at high temperature and pressure. The lower part of the rocket is the box we want to simulate. We assume that hot hydrogen is transferred from the combustion

chamber is such a manner that the density and temperature in the box is always constant despite the fact that hydrogen continuously escapes through the hole at the bottom.

Our task is therefore to simulate gas particles in the box and count the momentum Δp which is lost per time Δt . We know that force can be defined as

$$F = \frac{\Delta p}{\Delta t}$$

Knowing the force, we can find the acceleration from Newton's third law. As long as the density and temperature in the box is constant, the momentum loss will be constant and thereby the acceleration. Knowing the acceleration, we can therefore find the increase in velocity Δv gained after accelerating a given time ΔT . Note that the gas particles will escape and leave momentum in many different directions. But as the direction of the particles is random, only the momentum in the direction perpendicular to the area of the hole will produce a net force on the rocket. In all other directions the forces will cancel each other (do you see this?).

This is now in principle an easy task, given the simulation of particles in a box which you created in the chapter on pressure. However, in order to achieve realistic accelerations, the gas density and thereby the number of particles in the box would need to be far too high to make the simulation feasible on your own laptop. We therefore need to make one further simplification. This is shown in figure 6.

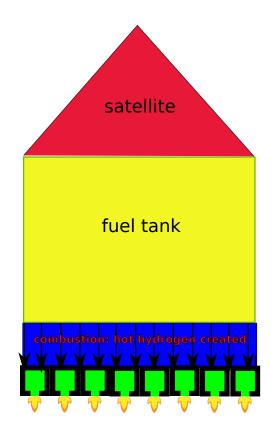


Figure 6: A simplified model of a rocket.

Instead of having one big box with a hole at the bottom of the rocket, we now substitute it with millions of tiny boxes, all with a hole. The size of each box will be fixed such that the simulation of one box becomes feasible on your laptop. Even with a high density, given a small box, the number of particles in the box will be limited. You now simply need to simulate one single tiny box and then multiply the momentum loss with the number of boxes. You will do this in exercise 1A.6. In that exercise you will show that using millions of tiny boxes instead of one big box gives exactly the same result, as long as the pressure and temperature of the gas is the same and the total area of all the holes in the small boxes corresponds to the area of the single hole in the big box. Using tiny boxes is therefore only a trick that we use in order to be able to calculate the thrust of our simplified rocket engine in figure 5.

The goal of the exercise will be to accelerate your rocket to the escape velocity of your home planet.

The escape velocity is the velocity needed for the kinetic energy to be larger than the potential energy such that the satellite is free from the gravitational potential of the planet. In order to find the escape velocity we therefore need to equal the kinetic and the potential energy:

$$\frac{1}{2}mv_{\rm esc}^2 = G\frac{mM}{R}$$

where m is the mass of the satellite, M is the mass of the planet and R is the distance from the center of the planet to the rocket, in this case the radius of the planet. We thus have

$$v_{\rm esc} = \sqrt{\frac{2GM}{R}}$$

Inserting the mass and radius of earth, we find that the escape velocity from the surface of the Earth is $v_{\rm esc} \approx 11 {\rm km/s}$.

Now you are ready to do exercises 1A.6 and if you wish also 1A.7

6 Exercises

Exercise 1A.1 You should read section 1 before doing this exercise. In this and the coming exercises you will need to do numerical integrations. Prepare your favorite numerical integration algorithm.

We will look at some temperature statistics. In order to make it easy we will focus on a tropical country where the mean temperature is basically constant all year. The mean temperature (averaged over day and night) in Kuala Lumpur is about 29 degrees all year. Assume that the fluctuations of the temperature from day to day is Gaussian distributed with a standard deviation of 2.

- 1. Calculate the probability that the mean temperature in Kuala Lumpur tomorrow is above 30 degrees?
- 2. Calculate the probability that it is between 27 and 31 degrees? (hint: no numerical integration needed).
- 3. Calculate the probability that the mean temperature in Kuala Lumpur is above 30 degrees every day for the next 7 days? Assume that temperature one day does not influence the temperature of the following days.
- 4. Calculate the probability that the temperature is above 30 degrees during 4 of the next 7 days, and below 30 degrees the remaining 3 days?

Exercise 1A.2 You should read section 1 before doing this exercise. Here we will look at data for rainfall in Sydney during the period 1885 to 1998. Download the file

http://www.uio.no/studier/emner/matnat/astro/ AST2000/h18/undervisningsmateriell_h2018/ data_og_filer_til_oppgaver/filer-til-oppgaver-i-del-1a/ sydney_rainfall_data.txt

with the relevant data taken from the Australian Bureau of Metereology. The first column shows the year, the next 12 columns the yearly rainfall in mm month by month for the given year. The final column shows yearly rainfall. Before starting this exercise, write the beginning of a python

code where you read these data.

- 1. The purpose of this exercise is to write your own python code to make a histogram. Please resist the temptation to use existing python commands for making histograms: you may gain some more intuition into the meaning of distributions by writing this code yourself.
 - (a) Choose one month and make an array with the rainfall for this month, year by year.
 - (b) Define 20 equally spaced bins between the smallest and largest value in your list (for instance if your values range from 100mm as the smallest rainfall to 200mm as the largest, you get the bins 100mm-105mm, 105mm-110mm, 110mm-115mm etc.)
 - (c) Now make the code which counts, for each bin, how many years which have a rainfall corresponding to the given bin. For each bin you get the number of years with corresponding rainfall.
 - (d) You now have a probability distribution of rainfall for the given month. But in order for this to be proper probabilities, your distribution needs to be normalized. Find our how (and if you can't, read section 1 again).
 - (e) Plot your histogram, middle of the bin on the x-axis (for instance 102.5mm, 107.5mm, etc) and probability on the yaxis.
 - (f) Is the rainfall distribution Gaussian?
 - (g) Try another month. Is the histogram equal?
- 2. Calculate the mean rainfall month by month. First by the standard method: simply take the mean of all the numbers for that month. Then by the method in equation 4, rewriting the integral as a sum over your bins. What is your probability *P* which you need to do this calculation?
- 3. Calculate the standard deviation month by month. Again, use both methods.

- 4. Now we will see if the central limit theo- need the following relations: rem may be valid for the rainfall statistic. Year by year, take the mean rainfall over all months for that year. In this way you get the average rainfall per year. Use your histogram code to make a histogram. Does it look more Gaussian?
- 5. Calculate the mean and standard deviation and insert these in the formula for the Gaussian distribution. Plot it on top of the histogram. Now you can get a better test of how Gaussian your histogram looks like. It should look much more Gaussian than the original month-by-month histogram, but it will not be a perfect Gaussian. Can you find at least 2-3 reasons why this is the case?

Exercise 1A.3 Now that you have got some experience in using probability distributions, we will deduce some of the results from the text.

- 1. Use your numerical integrator to show the probability for an event to be within 1σ , 2σ and 3σ of the mean of a Gaussian distribution. The results are given in the text. Now find also the probability to be within 4σ of the mean.
- 2. Show equation 2 analytically by using the definition of FWHM and playing with the expression for a Gaussian.

Exercise 1A.4 You should read sections 1 - 2 before doing this exercise. Again you need numerical integration.

- 1. The density and temperature in the core of the Sun is $\rho = 150 \times 10^3 \text{kg/m}^3$ and T = 15million K. Assume that the gas is ideal and consists of pure hydrogen. How many hydrogen particles per m³ have a total velocity between 100 m/s and 1000 m/s?
- 2. How many particles per m³ have a velocity between 100 m/s and 200 m/s in the x and y directions and a velocity between 100 m/s and 1000 m/s in the z-direction?

Exercise 1A.5 You should read sections 1 - 4 before doing this exercise. In this exercise, all calculations should be done analytically. You will

$$\int_0^\infty dx e^{-x} x = 1$$

and

$$\int_0^\infty dx e^{-x} x^{3/2} = \frac{3\sqrt{\pi}}{4}.$$

- 1. Find an expression for the mean absolute velocity of a particle with mass m in a gas with temperature T. You can start from equation
- 2. Deduce the equation of state for an ideal gas. Start from equation 12.
- 3. Show analytically that the mean kinetic energy of a particle in a gas of temperature Tis

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

Remember that the kinetic energy of a particle is given by $\frac{1}{2}mv^2$. Using that combined with what you have now learned about statistics and gases you should have all the information you need to solve this exercise.

Exercise 1A.6 You need to have read all of part 1A in order to be able to solve this exercise. In this and the following exercise you will need to access your solar system through the SolarSystem class in the ast2000tools package. The only information you need here is the mass of your home planet (your home planet is the planet with index 0). Note further that there are skeleton codes available on the course web page to help you with these two exercises (but if you manage to write the code from scratch yourself, that would be even better). Included in one of the code skeletons is a plotting example which you can use to animate the particles in your box in order to check that they behave as expected. To prevent the animation from being too slow, use very few particles (maybe about 100). When you see that the movement of the particles seems correct, you can continue coding, increasing the number of particles to at least $N = 10^5$ as explained below.

In this exercise you will create a rocket engine to make a satellite escape the gravitational potential of your home planet. Your task is to create a simplified rocket engine which can accelerate a satellite with the weight of 1000 kg (plus the weight of the fuel which we will ignore for the moment) to escape velocity. Assume the size of your box is $L = 10^{-6}$ m, the temperature of the gas is T = 10000K and the number of particles in the box $N = 10^5$. Assume all gas particles are hydrogen molecules H_2 . We will do this step by step:

- 1. Calculate the escape velocity $v_{\rm esc}$ for your home planet.
- 2. Start the code by creating two arrays, one with the (x, y, z) positions of all N particles and another with the (v_x, v_y, v_z) velocities of all N particles. Draw these positions and velocities from their respective distributions as described in the text (yes, you do need to read and understand all sections before you embark on this exercise).
- 3. Having created the random particle positions and velocities, you can now use this to check (a) if the mean kinetic energy of the particles in the gas is really (3/2)kT and (b) that the mean absolute velocity of the gas particles really follows the expression you found in exercise 1A.5. How good is the agreement with the analytic expressions? This is an important test of consistency to see that your gas velocities have been correctly set up.
- 4. Now we are ready to test the pressure of the gas.
 - First look at one particle with its given velocity and think how this particle will continue moving, How can you find the new position of this particle after a short time step?
 - When you have realised this, move all the particles during a **total period of** $\Delta T = 10^{-9}$ seconds with 1000 time steps (**each step of** $\Delta t = 10^{-12}$ **seconds**) during this period (you may try with longer or shorter periods and time steps).
 - At each time step, check for particles which hit each of the walls in the box.
 - Draw a particle with a given velocity vector on the way to collide with one

- if the walls. Draw the velocities, momentum, force and then how the new momentum and velocities need to look like after the collision, assuming it was elastic.
- Correct positions and velocities for all particles colliding during this time step assuming elastic collisions (see again the text). Make sure the particles do not continue to move outside the walls of the box.
- 5. In order to measure the pressure, we need to count the force that the particles exert on the walls.
 - (a) Choose one of the walls in your box and count all particles which collide with this wall during ΔT . Count the momentum that they leave on the wall (you may use some help from the text). Having the momentum and the time period, calculate the gas pressure in the box
 - (b) Compare with the analytic pressure you get from the equation of state. How good is the agreement?
- 6. Looking back to section 5 it is easy to see that we almost have our rocket engine simulation ready. All you need to do now is to make a hole in the box. To make it easy, just use the same wall as you used to measure pressure. Make a quadratic hole of length L/2 and count all the particles which escape the hole. Note that you will need to count (a) the momentum (in which direction?) and (b) the number of particles escaping. The first will be used to calculate the acceleration the rocket gains, the second to calculate the corresponding fuel loss. For simplicity we will assume that the fuel consists solely of hydrogen and that the total fuel loss corresponds to the total mass of fuel you need to bring. Note that in order for the density in the box to remain constant, the box is constantly being refilled from the combustion chamber above. How can you include this in the code? There is an extremely easy way and a slightly more complicated way. Which one do you choose? (no hints here)

- 7. Use the momentum loss to calculate the total speed gain Δv of the box (and thereby of the satellite) after the period ΔT .
- 8. In order to get the rocket to escape velocity within less than 20 minutes of acceleration, what is the minimum number of boxes needed for the rocket engine? Ignore fuel loss and the gravitational pull during acceleration.
- 9. How much fuel do you need to accelerate your 1000 kg satellite to escape velocity? You have made two very inaccurate approximations: you did not include the fuel mass in the calculation and you ignored the gravitational pull during acceleration. We will look into this in the next exercise.

Exercise 1A.7 This exercise builds on the previous exercise. You should have finished that exercise first. In this exercise we will take into account the mass of the fuel as well as the gravitational pull during acceleration. The goal is to find the density and temperature of the gas in the rocket engine necessary in order for the satellite to reach escape velocity within 20 minutes of launch.

- 1. First of all: thinking about the way you calculate the pressure, comparing it with the way you calculate the momentum loss and remembering the equation of state you should now realize that you can actually calculate the acceleration of the rocket in one given time step analytically using the equation of state. Do you see how?
- 2. Knowing the momentum and mass loss of your rocket engine (box), we can try to simulate the full acceleration of the rocket using the same engine as in the previous exercise. Find a suitable number of time steps between 0 and 20 minutes. Start with the full mass equal to the mass of the satellite plus the mass of the fuel which you calculated in the previous exercise. At each time step evaluate the speed gain Δv as well as the updated total mass of the rocket. Now you need to take into account the gravitational acceleration $\Delta v = -(GM_{\rm planet}/r^2)\Delta t$ at each time step. Which speed did you reach after 20 minutes? Clearly you did not

- reach escape velocity as the total mass was larger than in the previous exercise.
- 3. Now go back and adjust density (size of box), temperature, amount of fuel and the number of boxes in order to just reach escape velocity after 20 minutes. Here you have to do a combination of thinking, trial and error to understand what influences the thrust of the engine and simulations. In this exercise it is important that you thoroughly describe your full line of reasoning, all the tests you did in order to find a solution, why you did them and how. Your goal is to reach escape velocity with the smallest possible use of resources (i.e. the lowest fuel consumption and gas temperature that you can manage). Also think about the full area of the hole, is it realistic? If your home planet is very heavy, you may have to use less realistic temperatures and/or hole sizes to reach your goal.

Exercise 1A.8 You need to have read all of part 1A in order to be able to solve this exercise. We will now study a very simplified model of star formation. You will learn more details about star formation later in this course, but here we will make a small simulation: A star normally starts out as a cloud of gas, a cold molecular cloud which collapses gravitationally. These clouds normally have temperatures between 10K and 50K. As the gravitational collapse starts, the temperature increases untill the central parts of the cloud reach temperatures of a few million Kelvin when nuclear reactions start.

Ideally, in order to simulate the gas cloud, one should simulate the movement of each single molecule. Being infeasible, we will divide the gas cloud into N particles and follow the movement of each of these particles assuming they behave as gas particles. If the total mass of the cloud is M, each particle will have mass $M_{\rm part} = M/N$ in order to conserve the real gravitational pull on the particles. Note that since the gravitational acceleration of the particles in the cloud is independent of the mass of the particle (why?), the movement of our macroscopic particles will be similar to that of the gas particles making our approximation reasonable for some purposes.

In the following link, you can find a list of initial particle positions and velocities in 3 dimensions for 500 particles:

http://www.uio.no/studier/emner/matnat/astro/ AST2000/h18/undervisningsmateriell_h2018/ data_og_filer_til_oppgaver/filer-til-oppgaver-i-del-1a/ gas_cloud.txt

Each of the 500 lines have 7 columns: the first is particle number, then the three spatial positions (x, y, z) in meters and finally the three velocity components (v_x, v_y, v_z) . We will assume our cloud to have exactly the mass of the Sun. Load particle positions and velocities. For each particle you now have a position vector $\vec{r} = (x, y, z)$ pointing to the position of the particle from the origin and a velocity vector $\vec{v} = (v_x, v_y, v_z)$. In the following exercises, when calculating the gravitational forces, we need to use the fictive mass $M_{\text{part}} = M/N$ for the particles. However, when computing the properties of the gas (i.e. temperature), we will assume these particles to be hydrogen atoms with mass $m_H = 1.67 \times 10^{-27}$.

- 1. Calculate the mean kinetic energy of the particles in the gas and use this together with an expression from exercise 1A.5 to find the temperature of the gas.
- 2. For each dimensions x, y and z, make a histogram of gas velocities v_x , v_y and v_z . On top of these three plots, plot the Maxwell-Boltzmann distribution function for the temperature which you found in the previuos question. Do they fit? Did you expect them to fit?
- 3. The particle positions are all within a sphere if radius 2.5×10^{11} m. In order to calculate the gravitational pull on each particle, we need to divide this sphere into 100 shells with equal thickness Δr . You should already have arrays for positions x, y and z as well as velocities v_x , v_y and v_z for all particles. You should now write a code to calculate (a) the distance from the center (in meters) and (b) the shell number (from 0 to 99) for each particle and store these in arrays (with dimension 100).
- 4. You should now write a code which calcu-

lates the number of particles present in each single shell and store these in an array.

5. We will now write a code to calculate the gravitational pull on a given particle from all the other particles. If we assume the particles to be homogeneously distributed on a sphere (which is a good approximation here), then all particles in shells outside our given particle will not contribute to the gravitational pull on the particle. This is true as it can be shown that the gravitational pull on an object inside a homogeneous spherical shell is zero. We therefore need to calculate the gravitational pull from the sphere inside the given particle. The gravitational pull is therefore

$$\vec{F}_g = -G\frac{M(r)M_{\text{part}}}{r^3}\vec{r}$$

where r is the distance to the particle from the center, \vec{r} is the position vector of the particle, $M_{\rm part}$ is the mass of the particle and M(r) is the total mass of the sphere inside the particle. For a given particle your code therefore needs to find (a) the total number of particles in the sphere inside the position of your particle summing over all shells inside your particle's shell, (b) the force vector \vec{F}_g by combining the result in (a) with the values for r and \vec{r} (which you should already have). Note that if the particle is in the innermost shell, we assume that no force is working on it.

6. As the particles start accelerating inwards, there are several processes which will slow down the particles and thereby cool the gas: (1) Charged accelerated particles start radiating, (2) as the gas density increases, the particles will start colliding and (3) as the particles reach thermal equilibrium they will start radiating Planck radiation. In order to mimic these complicated effects, we will add a friction term by simply assuming that the particles loose velocity depending on the relative density of their shell as well as their absolute velocity $|\vec{v}|$:

$$\frac{\Delta \vec{v}_{\rm fric}}{\Delta t} = -K\rho |\vec{v}|\vec{v}$$

where $K = 1.3 \times 10^{-9} \text{m}^{-1}$, $\rho = N_{\text{shell}}/N$ where N_{shell} is the total number of particles in the same shell as the particle and N is the total number of particles in the cloud.

- 7. Use Newton's second law to write a code to calculate the acceleration vector \vec{a} of a given particle using the force from gravitation. In the acceleration you should also take into account the density dependent deceleration.
- 8. We will now use Euler's method to update the velocity and position for each particle. In part 1B, you will learn more about Euler's method, here we will make a simpler explanation: We need to find the change $\Delta \vec{v}$ in the velocity vector. Knowing that accelaration is just $\vec{a} = \frac{\Delta \vec{v}}{\Delta t}$, we can write

$$\Delta \vec{v} = \vec{a} \Delta t$$

Use a time step of 10^{-5} year and write a code to update the velocity \vec{v} of a given particle.

9. Having updated the velocity, we can now update the position of the particle. We know that velocity is just change of position per time, $\vec{v} = \frac{\Delta \vec{r}}{\Delta t}$, giving

$$\Delta \vec{r} = \vec{v} \Delta t$$

Use again a time step of 10^{-5} year and write a code to update the position \vec{r} of a particle.

- 10. Now we are ready to write the full code: Loop over 7×10^4 time steps. For each time step, loop over all particles. Depending on how poweful computer you are using, you could start using only the first 50 particles, and adjusting the particle mass accordingly. When your code runs well, you may increase the particle number if the code is sufficiently quick. Otherwise, stick to 50 particles. For each particle, update velocity and position.
- 11. When position and velocity for all particles have been updated for the given time step, make another loop on particle and update the arrays for distance r from the center and shell number for each particle. For the particles which pass from one shell to another, you also need to update the array keeping track of the number of particles in each shell.

- 12. For each time step, calculate and save the new temperature and mean radius of the cloud. In order to find the mean radius, you can just take the mean over the distance r from the center to all of the particles. However, you may have a situation where a few of the particles leave the gas cloud and should thereby not be used in calculating radius and temperature of the cloud. Try to find a way to take this into account.
- 13. You may make a movie of the collapse by dumping a png of your cloud every 500 time steps. You may use the relevant part of the skeleton code for exercise 1A.6.
- 14. After the collapse, plot the radius of the cloud as a function of time. Has the contraction stopped, or does it still collapse?
- 15. Find the new radius of your gas cloud and compare it to the radius of the Sun. Do you expect the collapse to have finished?
- 16. Plot the gas temperature of the cloud as a function of time. Does the temperature seem to have converged? Is temperature a smooth function of time? If not, what could be the reason? If the problem is numerical, what could you do to improve the temperature values?
- 17. Use the plot to estimate the temperature of the cloud at the end of the simulations (how?). You need several million Kelvins in order to start nuclear reactions. Is the star fully formed at this stage?
- 18. Make again histograms of the velocity distributions and compare to Maxwell-Boltzmann. Is this still an ideal gas or did something change during the collapse?
- 19. Compare your current mean radius of the cloud to the radius of your innermost shell. You should find that these are similar. Can you explain why? Do you think the cloud will collapse further? Why/why not?
- 20. The total real time of your simulation is 0.7 years? Check how much the cloud has collapsed and how much the temperature has increased in such a short time scale. Is this realistic? If not, what did we do wrong?

21. Now you should rerun the whole simulation, but remove the density dependent decceleration. Explain what you think will happen

and why. Then make a movie of the process and compare to your expectations.