Astrophysics with the Computer: Evaporation/Condensation of Gas Clouds

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1 Warning

This exercise is very experimental. Your work and your experiences will help to better define this exercise. Your spotting mistakes and any comments are welcome.

2 Astrophysics

What happens to a small cloud of cool dense gas when it is embedded in a dilute and hot medium? Since thermal conduction will transport energy from the hot medium to the cool gas, the cloud will often simply evaporate, but under certain conditions, the hot gas could cool and condense onto the cloud. The question of the fate of such a cloud occurs in several contexts:

- stellar winds driven by radiation pressure by a hot star are known to be clumpy. How long do these clumps survive?
- the interstellar medium is a mixture of neutral clouds and hot ionized gas. What happens to the clouds when the physical conditions change, such as by the passage of a spiral arm, star formation in clouds, the production of hot gas by supernova explosions? What is the 'normal' state of this multi–phase interstellar medium?
- the hot gas captured by the gravitational field in galaxy clusters is neither homogeneous. If some part of the gas is dense enough to cool down, it will start moving towards the massive cD galaxy in the centre. As it gets denser it will cool more rapidly, and eventually, there is a current of gas moving towards the centre while cooling (a "cooling flow")
- matter in the Universe is not distributed perfectly homogeneously, so there are denser cooler regions next to dilute hotter regions. How do they evolve?

This exercise deals with the fate of a small, spherical ball of gas surrounded by dilute but hot gas, in pressure equilibrium. Thermal conduction and radiative cooling will be considered to find out what happens to the cloud.

A number of works have dealt with this problem. The results of Cowie & McKee (1977) and McKee & Cowie (1977), who did some semi–analytical studies, are widely used in various contexts. Recently, Wolfgang Vieser, one of our Ph.D. students in Kiel, has done 2–dimensional numerical calculations of the full problem, and finds that the formulae given by Cowie and McKee do not give the same results. Let us do some simple model to check Cowie and McKee!

3 The equations

We consider a spherical cloud, so we need to solve the equations only in the radial direction, and we have a 1–dimensional problem only. The conservation of mass becomes

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^2}\frac{\partial r^2 v \rho}{\partial r} = 0 \tag{1}$$

because there shall not be any gas entering from the outside or leaving our region of computation.

The cloud shall be small, so that we can neglect its own gravity, which would make things a bit more complicated. So the conservation of momentum has only the pressure gradient

$$\frac{\partial \rho v}{\partial t} + \frac{1}{r^2}\frac{\partial r^2 \rho v^2}{\partial r} = -\frac{\partial p}{\partial r} \tag{2}$$

The pressure $p = k_{\mathrm{B}} T \rho / m_{\mathrm{g}}$ is taken for an ideal gas with mean molecular weight m_{g}. If you really wanted to include self–gravity, we need to add the term $-(G\rho/r^2)4\pi \int_0^r \rho(r')r'^2 dr'$ to the right hand side of the momentum equation. But this involves computing another integral.

In the equation for the energy density $e = 3p/2$ (ideal gas)

$$\frac{\partial e}{\partial t} + \frac{1}{r^2}\frac{\partial r^2 e v}{\partial r} = -\frac{p}{r^2}\frac{\partial r^2 v}{\partial r} + H - C - \frac{1}{r^2}\frac{\partial r^2 q}{\partial r} \tag{3}$$

we have on the right hand side the $p\Delta V$ work, gains by heating, losses by cooling, and thermal conduction.

We shall neglect any heating $H = 0$ by e.g. stars, cosmic rays etc. as this would depend on the specific environment, but we probably need something in order to keep thermal equilibrium for the initial configuration. The cooling rate is due to radiation of optical, IR, and radio lines and continua, in which the cloud and the ambient medium is completely transparent, so that every photon produced is lost. One has:

$$C(\rho, T) = \rho^2 \Lambda(T) \tag{4}$$

For a collisionally ionized gas, Böhringer & Hensler (1989) have computed from basic atomic physics Λ as a function of temperature. I suggest, that you use the curve for solar metallicity ($Z = 0.02$), and invent a suitable analytical formula to fit the published curve reasonably well (factor 2 or better).

The energy flux q due to heat conduction we take from Spitzer (1962)

$$q_{\mathrm{classic}} = -\kappa \cdot \frac{\partial T}{\partial r} \tag{5}$$

with the thermal conductivity

$$\kappa = \frac{1.84 \cdot 10^{-5}\, T^{5/2}}{\ln \Psi} \qquad \mathrm{erg\,s^{-1}K^{-1}cm^{-1}} \tag{6}$$

and the Coulomb logarithm

$$\ln \Psi = 29.7 + \ln \left[\frac{T_e/10^6\,\mathrm{K}}{\sqrt{n_e}} \right] \tag{7}$$

with the temperature $T_e = T$ and density $n_e \approx n_{\mathrm{protons}} \approx \rho/m_{\mathrm{p}}$ of the electrons, which are responsible for the heat conduction. This classical expression breaks down when the electron mean free path becomes comparable to the temperature scale height. Therefore, one limits the flux q by the so–called "saturated" heat flux

$$q_{\mathrm{sat}} \approx 5\rho c_s^3 \tag{8}$$

where c_s is the isothermal sound speed, and one makes a smooth transition between the two formulae by

$$q = q_{\mathrm{sat}} \left(1 - \exp \left[\frac{q_{\mathrm{classic}}}{q_{rmsat}} \right] \right) \tag{9}$$

4 Evaporation rates

Cowie & McKee (1977) studied the problem analytically, and they found that a cloud of radius R will evaporate with a mass–loss rate

$$\dot{M} = \frac{16\pi m_{\mathrm{g}} \kappa_f R}{25 k_{\mathrm{B}}} \tag{10}$$

when we are in the 'classical' regime, where $q = q_{\mathrm{classic}}$. When they also take into account radiative cooling, they find that the cloud evaporates with the classic rate (if $0.03 < \sigma_0 < 1$) or the saturated rate ($1 < \sigma_0$), but gas condenses onto the cloud if $\sigma_0 < 0.03$. This depends on the saturation parameter

$$\sigma_0 = \frac{0.08\kappa_f T_f}{\rho_f c_f^3 R} = \frac{12300 T_f^2}{n_{ef} R} \tag{11}$$

which is essentially the ratio of electron mean free path to the cloud radius. The quantities with suffix f pertain to the undisturbed ambient medium.

How can we check this numerically? There are two possibilities which are as follows.

4.1 Steady–State Solution

Since we are interested in the mass–loss rate only, we could limit ourselves to finding the stationary solution only, if it exists. Physically, we are not looking at what happens to the cloud once we put it into the hot gas... as it evaporates, it looses mass, it gets smaller, until it may completely vanish. Clearly this is not a stationary situation! But we can imagine one, for e.g. evaporation: if we supply fresh gas to the cloud centre, it will stream towards the surface where it will stream into the hot gas, thereafter the hot gas streams further outside. If we construct such a model, we can measure the steady–state mass loss–rate towards which the (time–dependent) mass–loss rate of a eventually vanishing cloud will tend to.

Analytically, we look for solutions of the equations 1, 2, and 3 if the time derivatives are neglected. Let us do this for the Eqn. 1. Obviously this implies that

$$r^2 \rho v = const. \tag{12}$$

which expresses merely the fact that we look for a solution with a mass–loss rate $\dot{M}(r) = 4\pi r^2 \rho(r) v(r)$ which must be constant throughout the computational volume. Together with the feeding in of the appropriate amount of gas at the clouds centre (for evaporation) and its drainage in the hot gas far away from the cloud, this is the imaginary model we want to consider.

Unfortunately, the other two equations are too complicated to find an analytic solution. But we can tackle them numerically: Given the conditions at the cloud centre, we can integrate them in radial direction until we reach the hot gas. There we check whether the solution obeys the assumed physics. This is the basic idea.

4.1.1 Isothermal Case

Before we tackle the whole problem, it is better to consider a simpler case. If the gas were isothermal, we do not need the energy equation. We get from Eqn. 2

$$\frac{1}{r^2}\frac{dr^2 \rho v^2}{dr} = -\frac{dp}{dr} = -c_s^2 \frac{d\rho}{dr} \tag{13}$$

with the isothermal sound speed $c_s = \sqrt{k_{\mathrm{B}} T / m_{\mathrm{g}}}$. Since we look for a solution with constant $\dot{M}$, we can write

$$\frac{dr^2 \rho v^2}{dr} = \frac{d\dot{M}/4\pi v}{dr} = \frac{\dot{M}}{4\pi}\frac{dv}{dr} \tag{14}$$

which gives a differential equation for the streaming velocity

$$\frac{dv}{dr} = -\frac{4\pi r^2 c_s^2}{\dot{M}}\frac{d\rho}{dr} \tag{15}$$

From the mass conservation, we then get the density

$$\rho = \frac{\dot{M}}{4\pi r^2 v} \tag{16}$$

Starting at the centre of the cloud, or at some small radius r_0 with $\rho_0 = \rho(r_0)$ and $v_0 = v(r_0)$, we can integrate the equation for the velocity and the density.

We can roughly predict how the solution would look like: The density would be largest at the centre, so the gradient $d\rho/dr$ will be negative. This means that the velocity increases. Far away from the cloud, the density in the hot region will be nearly constant, so the velocity does not increase further. But it cannot be constant, as we demand that $\dot{M}$ is constant, so the gradients dv/dr and $r^2 d\rho/dr$ will tend to zero in the same way.

The crucial question now is whether the density we get in the hot gas region (in the limit $r \to \infty$) is the one we had assumed for the hot gas! If it doesn't, soemthing in our model is wrong. This something are the initial conditions ρ_0 and v_0. While the cloud density ρ_0 is a parameter that must be kept free, the velocity v_0 is not free, because its value – given r_0 and ρ_0 – is determined from the mass–loss rate which is a **result** of the model. If we vary the assumed value for $\dot{M}$, so will the limiting gas density. The only interesting solution is the one where $\rho \to \rho_{\rm hotgas}$. If this value for $\dot{M}$ is positive, we have evaporation, if it is negative, we have condensation. In order to find out, we have to integrate the equations for various guess values of the mass–loss rate.

To do this by trial–and–error is a tedious way. In principle one could use the iterative Relaxation Method to find the solution. This is described in the script for the Internal Structure of a Star, and in the very useful book "Numerical Recipes" (available at the D.E.A. library), but it needs a lot of work, and the Evolutionary Method (see below) is much more fun!

4.1.2 The full problem

If we tackle the energy equation as well, everything becomes a bit more complicated, but the principle is the same. We start integration at the cloud centre with ρ_0, v_0, and T_0, and we look for the behaviour at large radii. Now $\rho \to \rho_{\rm hotgas}$ as well as $T \to T_{\rm hotgas}$ should be met, and we have $\dot{M}$ and T_0 for adjustement. The problem becomes a search in two dimensions.

For the treatment of the heating function H, see the section on Initial Conditions below.

4.2 Evolutionary Method

The other method is to evolve the complete system, starting from the initial conditions, and wait until it relaxes into the steady state solution. This method is more direct and easier to interpret intuitively, as one deals with the simulated behaviour of a physical system, but it require much more computing time, because we need to solve the partial differential equations with sufficient accuracy. It is often used for physical problems like ours, because it needs a code which is useable to simulate other physical problems, and it is more flexible, if one wants to add another process or effect. But there may be many problems with accuracy and false effects.......

4.3 Initial Conditions

These remarks apply to both methods! We are interested in finding the mass–loss rate of a cloud with given properties in hot gas of given properties. However, we need to ensure that the initial situation is physically consistent with that state. Otherwise, effects enter which we are not interested in.

The first requirement is that the cloud and the gas are in pressure balance. Otherwise, the cloud would either expand on its own or compressed by the hot gas. To do this, we demand that

$$\rho_{\rm cloud} T_{\rm cloud} = \rho_{\rm gas} T_{\rm gas} \tag{17}$$

This is evidently a condition between the initial parameters. If we specify the density and temperature of the cloud and the temperature of the gas, $\rho_{\rm gas}$ is no longer a free parameter.

The second condition is that all the gas everywhere should be in thermal equilibrium. Otherwise, the cloud gas could cool, so its pressure drops, and it gets compressed by the hot gas. We demand that in the initial configuration – if all the radial derivatives were held to zero – that the local heating and cooling rates cancel each other

$$H = C = \rho^2 \Lambda(T) \tag{18}$$

where T is the respective initial temperature. When the heating rate and the densities are given, the temperatures in the cloud and the gas would be fixed. But as we also demand pressure balance, we now cannot specify freely more than two parameters! This would limit the application of our results to that particular case only, and we cannot check the formulae of Cowie & McKee in all parameters. So, for the benefit of our liberty, we shall not try to make a realistic model of thermal and pressure equilibrium in the interstellar medium, but we shall fix H in the cloud and in the gas (separately) to whatever value is necessary to get the assumed temperatures from the assumed densities. But we must interpolate between cloud and gas: this we do by assuming some simple density and temperature dependence of

$$H = H(\rho, T) = H_0 \rho^x T^y \tag{19}$$

with x and y to be determined by this system of non–linear equations

$$\begin{aligned}
\rho_{\rm cloud} T_{\rm cloud} &= \rho_{\rm gas} T_{\rm gas} && (20)\\
H_0 \rho^x_{\rm cloud} T^y_{\rm cloud} &= \rho^2_{\rm cloud} \Lambda(T_{\rm cloud}) && (21)\\
H_0 \rho^x_{\rm gas} T^y_{\rm gas} &= \rho^2_{\rm gas} \Lambda(T_{\rm gas}) && (22)
\end{aligned}$$

where Λ is your analytical approximation of the cooling function. Do not make yourselves too much work here! A crude approximation may be enough (e.g. $y = 0$).

5 How to solve it numerically

5.1 Integration of Initial Value Problem

To integrate the equation $dy/dx = f(x, y)$ starting from the initial condition $y(x_0) = y_0$, we may employ a simple method, such as to apply for all $i = 1, ..., n$

$$y_i = y_{i-1} + f(x_{i-1}, y_{i-1}) \Delta x \tag{23}$$

with some suitably small step Δx which is here in radial direction.

You may also use more sophisticated methods, such as Runge-Kutta, which gives a more accurate solution for the same size of the stepwidth.

It may well be necessary to use a step Δx which is adapted to ensure a certain minimum accuracy. This usually is required when the slope $f(x, y)$ changes over a large range. One possible way is to demand that the relative increment in y must always be less than a certain value η:

$$\Delta x = \frac{\eta}{|f(x_i, y_i)/y_i|} \tag{24}$$

which is evaluated each time after the derivatives have been comoputed. But be careful: if $f \approx 0$ the step will be unhealthily large, and for very large f the step may be so small, that the program will not finish before you finish the D.E.A.

5.2 Finite Difference Method

We shall use the method of finite differences. This means that we divide space and time (here: radius and time) into many small intervals – the sizes of these intervals must be chosen so that one get a sufficient resolution. Thus, all the functions of the problem (here: density, temperature, velocity, etc.) are thus given only on these discrete points. All derivatives will be approximated by their differences on these grids. For example,

$$\frac{df}{dt} = \frac{f(t_2) - f(t_1)}{t2 - t1} \tag{25}$$

To solve the differential equation $dy/dt = f(y, t)$ we get a scheme to compute from the 'old' value $y(t)$ the 'new' value at one time-step later:

$$y(t + \Delta t) = y(t) + \Delta t \cdot f(y(t), t) \tag{26}$$

Note that we've used on the right-hand side only data that is known at the 'old' time, so we use an explicit method. The size of the time step Δt determines the accuracy of the calculation, obviously a smaller time-step makes it more accurate.

To solve a partial differential equation, we chose e.g. the simple explicit method above (which is a 1st order method) to do the time stepping. All other derivatives (in radius) are also computed from formulae of this type, but evaluated of course at the old time:

$$\frac{\partial}{\partial r} f(r_i, t) \approx \frac{f(r_i, t) - f(r_{i-1}, t)}{r_i - r_{i-1}} \tag{27}$$

This is a simple first order recipe, which might also cause problems, because it is asymmetrical in radial direction. The simple second–order scheme is symmetrical

$$\frac{\partial}{\partial r} f(r_i, t) \approx \frac{f(r_{i+1}, t) - f(r_{i-1}, t)}{r_{i+1} - r_{i-1}} \tag{28}$$

but it has an instability, because the derivative at radius i does not depend on the function at that point....

5.3 How to make differencing formulae

In a finite difference method we need formulae that approximate differential quotients by difference quotients. Here is a reminder how to make such a formula with a given order of accuracy:

Suppose I want to approximate the derivative in the central point x_2 by using three points of the grid (x_1, x_2, x_3), and I demand second-order accuracy

$$\frac{dy}{dx} \approx A \cdot y(x_1) + B \cdot y(x_2) + C \cdot y(x_3) \tag{29}$$

First, we express the function $y(x)$ by its Taylor series about the (desired) midpoint (with $h = x - x_2$):

$$y(x) = y_2 + h \cdot y_2^{(1)} + \frac{h^2}{2} \cdot y_2^{(2)} + \frac{h^3}{3!} \cdot y_2^{(3)} + ... \tag{30}$$

or

$$dy/dx = y_2^{(1)} + \frac{h}{2} \cdot y_2^{(2)} + \frac{h^2}{3!} \cdot y_2^{(3)} + ... \tag{31}$$

When we demand second-order behaviour

$$dy/dx = y_2^{(1)} + O(h^2) \tag{32}$$

this means that the term depending on $y_2^{(2)}$ should vanish. On the other hand, we evaluate the right hand side of Eqn. 29 putting in the Taylor expansions

$$\begin{aligned} dy/dx &= A(y_2 + h_{12} \cdot y_2^{(1)} + \frac{h_{12}^2}{2} \cdot y_2^{(2)} + ...) \\ &+ By_2 \\ &+ C(y_2 + h_{32} \cdot y_2^{(1)} + \frac{h_{32}^2}{2} \cdot y_2^{(2)} + ...) \end{aligned} \tag{33}$$

with $h_{ik} = x_i - x_k$. If this should be equal to Eqn. 32 up to 2nd order for any function $y(x)$, we get a system of linear equations for the coefficients A, B, C:

$$\begin{aligned} A + B + C &= 0 \\ A \cdot h_{12} + C \cdot h_{32} &= 1 \\ A \cdot h_{12}^2/2 + C \cdot h_{32}^2/2 &= 0 \end{aligned} \tag{34}$$

which gives

$$\begin{aligned} A &= -\frac{h_{32}}{h_{12}(h_{12} - h_{32})} \\ B &= -\frac{h_{12}^2 - h_{32}^2}{h_{12}h_{32}(h_{12} - h_{32})} \\ C &= \frac{h_{12}}{h_{32}(h_{12} - h_{32})} \end{aligned} \tag{35}$$

This is the generalization for the well known formula for an equi-spaced grid ($h_{32} = -h_{12} = h$):

$$\begin{aligned} A &= -\frac{1}{2h} \\ B &= 0 \\ C &= \frac{1}{2h} \end{aligned} \tag{36}$$

With this method one can derive formulae for any derivative at any point with any accuracy. Obviously one has to choose the number of points in accordance with the required accuracy!

5.4 The grids

For the discretisation in time, we shall take the simplest one, i.e. with a constant time-step. What size you need, depends on the accuracy you want, and is best found out by experiments. It should not be too large, as the program will tell you rather quickly by 'exploding' sooner or later.

For the discretisation in space, let us first try a simple radial grid with constant interval. Since the problem has a symmetry centre at the origin, and terms with $1/r^2$ will grow there beyond any limit, it might be a good idea to concentrate the grid towards the origin, e.g. use a grid equally spaced in $\sqrt{r}$ rather than the simple linear one. This means that one cannot use discretizaion formulae built for constant step size, or one transforms the problem into that space, by working not with radii, but with $\sqrt{r}$. I recommend that you try out various things. Which one do you find to be the best one???

For a method stepping explicitly in time, the Courant-Friedrichs-Levy condition must be obeyed, if the method should not explode. The time step dt must be smaller than the time required for the *fastest* element to cross a radial grid cell:

$$dt < \min_i |\frac{\Delta r_i}{v_i}| \tag{37}$$

Usually, one does not take the full time step, permitted by this formula. See what happens if you don't obey it!

5.5 Boundary conditions

In our problem there is no exchange of matter with the outside. So no gas flows across either boundary. We set $v = 0$ at both the innermost and outermost cells, disregarding the solution from the momentum equation.

Just an idea: If you had found a stationary solution with the direct integration method, you might feed the mass–loss flux at the inner boundary, and to see whether the time-evolution method also finds the solution with constant mass–loss rate everywhere?

5.6 Initial conditions

For the cloud we specify the radius, within which we set the density and temperature. Outside, we use the hot gas values. It may be wise to make the transition from cloud to ambient gas not too abrupt, because numerical methods HATE jumps!

5.7 Transforming the equations

Often, it is not numerically wise to solve the equation in its original form. We are dealing with a problem with spherical symmetry. So the conservation of mass can also be written as

$$\frac{\partial r^2 \rho}{\partial t} + \frac{\partial r^2 \rho v}{\partial r} = 0 \tag{38}$$

So we might use $r^2\rho$ as a function instead of ρ.

5.8 Conservative Formulation

The way I've written the Eqns. 1 and 2

$$\frac{\partial A}{\partial t} + \frac{1}{r^2}\frac{\partial r^2 v A}{\partial r} = S_A \tag{39}$$

emphasizes that A is a conserved quantity (in rotationally symmetric coordinates). The second term is called advection; it counts how much of A is transported from and into a volume by the velocity v. The term on the right is a source term, telling how much is locally produced (or destroyed) of A. By formulating a discretisation recipe which ensures the balance of the three terms, one can build a code which strictly conserves quantity A. Here one would need a scheme in which all that is computed to leave radial element i with a positive velocity is equal to what is computed to arrive at radial element $i+1$, its neighbour.

6 Tasks

Here are some suggestions how to proceed:

- try out the direct integration method to find the stationary solution....
- ... but test your integration method carefully with a simpler equation whose analytical solution you know

- perhaps you just tackle the isothermal case to find out how the limiting density depends on the mass–loss rate. Do not spend too much time on the 2–D problem!
- if the direct integration does not work nicely, then you better try the time–evolution
- when you are able to compute the stationary solutions, do this for various physical parameters (densities, temperatures, cloud radius) so that you can compare your mass–loss rates with Cowie & McKee
- by a suitable scan of the parameters, we should be able to check the validity of the criterion with σ_0
- if you want to reproduce Cowie & McKee more precisely, one should also use exactly their recipes (cooling function)

7 Literature

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