Arthur Dromard: dromard@th.physik.uni-frankfurt.de
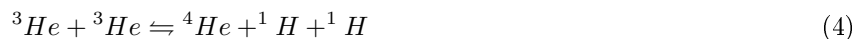
Nuclear reactions inside stars

1   Introduction

This project has two aspects: one physical and one numerical. The idea of this project is to simulate a star using a simplified model of nuclear reaction chain. Beyond this physical aspect, this is the opportunity to learn how to solve coupled differential equations numerically and to write your first simulation program from scratch. This presentation document is organized as follow: the first part is an introduction to physical aspects of the projet, that means the description of the model. And the second part is the instructions and advices for the programing.

2   The physical model

2.1   Introduction to the model

A star can be seen as a huge ball of gas. Large enough that its own weight allows the gravity to overcome the electric repulsion between two hydrogen nuclei. When these two hydrogen nuclei are close enough, they fuse. This is the beginning of a series of nuclear reactions which are prime energy producers in the sun. In the early life of a star (actually this is the longest period of its life $\cong 5$ billion years), the nuclear reactions are essentially those in the proton-proton chain which starts from proton (or hydrogen nucleus ^1H), creates deuterium, D , then helium 3, ^3He and finally helium 4, ^4He. The different steps of this chain are the following:

$$^1H + {}^1H \rightleftharpoons D + e^+ + \nu_e \tag{1}$$

$$e^+ + e^- \rightleftharpoons 2\gamma \tag{2}$$

$$D + {}^1H \rightleftharpoons {}^3He + \gamma \tag{3}$$

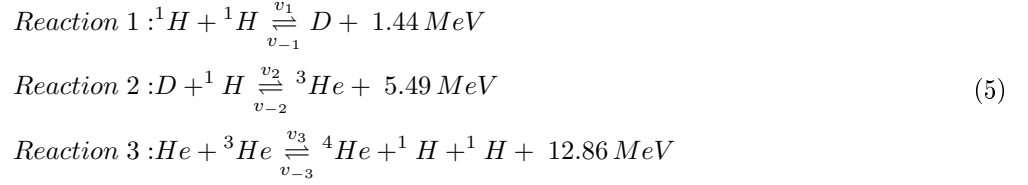$$^3He + {}^3He \rightleftharpoons {}^4He + {}^1H + {}^1H \tag{4}$$

Each reaction is an equilibrium. That means that you can go from left to the right or from right to the left. From left to the right the reactions are exothermic, that means that they create energy. From right to left the reactions are endothermic that means that they consume energy. The idea of the project is to create a small program which will simulate those reactions and from them get the energy which is radiated by the star due to those reactions.

2.2   Simplification of nuclear reaction

The idea is to compute the density of each particle as a function of time, starting from an initial condition and considering the previous reactions ((1) to (4)).

In our simple model the number of positrons (e^+), electrons (e^-), neutrinos (ν) are not relevant. They will be considered as energy. This is an important simplification that can be explained as follow. Let us start with the positron and the electron. The positron is the anti-particle of the electron, that means that they annihilate each-other creating energy. As the concentration of electrons is important and the annihilation reaction is really fast, each positron created are immediately annihilated and you can only observe the energy created by this reaction. The neutrino is another problem. This particle has almost no mass and interacts weakly. So when this particle will be created, it will escape from the star and so it can be seen as some energy radiated. Moreover its energy contribution is small compared to the energy contribution of the other elements so they can be completely neglected.

In consequence, the reactions can be rewritten as:

$$Reaction\ 1:{}^1H + {}^1H \underset{v_{-1}}{\overset{v_1}{\rightleftharpoons}} D +\ 1.44\,MeV$$

$$Reaction\ 2:D +{}^1H \underset{v_{-2}}{\overset{v_2}{\rightleftharpoons}} {}^3He +\ 5.49\,MeV \tag{5}$$

$$Reaction\ 3:He + {}^3He \underset{v_{-3}}{\overset{v_3}{\rightleftharpoons}} {}^4He +{}^1H +{}^1H +\ 12.86\,MeV$$

where v_i is the velocity of the reaction (this velocity depends essentially on the density of elements and on the temperature).

2.3 Equations of our model

Now that we have our reactions, we can express the variation of the number of nuclei with time using the previous reactions and their kinetics:

$$\begin{aligned}
\frac{dN_H(t)}{dt} &= 2\,(v_{-1} - v_1) + v_{-2} - v_2 + 2\,(v_3 - v_{-3})\\
\frac{dN_D(t)}{dt} &= v_1 - v_{-1} + v_{-2} - v_2\\
\frac{dN_{{}^3He}(t)}{dt} &= v_2 - v_{-2} + 2\,(v_{-3} - v_3)\\
\frac{dN_{{}^4He}(t)}{dt} &= v_3 - v_{-3}
\end{aligned} \tag{6}$$

As in our model, we suppose that all the energy is created by the proton-proton chain, the variation of energy can be expressed in the same way but this time we also have to take care about the energy lost by the black-body emission given by the Stefan-Bolzmann law, which is the last term of the following equation:

$$\frac{dE(t)}{dt} = (v_1 - v_{-1}) * E1 + (v_2 - v_{-2}) * E2 + (v_3 - v_{-3}) * E3 - \sigma * S * T^4 \tag{7}$$

where $E1$ is the energy of the first reaction ($1.44\,MeV$), $E2$ of the second ($5.49\,MeV$), $E3$ of the third ($12.86\,MeV$), σ is the Stefan-Bolzmann constant (Radiance of black body), S the surface and T the temperature.

In our simplified model, we can express the temperature as follow:

$$T(t) = \frac{E(t)}{N_0 k_B} \qquad \text{with} \qquad N_0 = N_H(0) + N_D(0) + N_{{}^3He}(0) + N_{{}^4He}(0). \tag{8}$$

We will also assume that our volume is fixed and can be represented as a perfect sphere. So the surface is

$$S = (36\pi)^{\frac{1}{3}} V^{\frac{2}{3}} \tag{9}$$

At this point, the only unknown element in our differential equations is the velocity of the equation: here we will work on two models, one really simple where the temperature dependence will be neglected and the second one more realistic where the temperature will be taken into account.

2.3.1 Basic model for velocity

In fact, our two models will differ theoretically only by the expression of the velocity. For the basic one, we will consider only the concentration dependence of the velocity and neglected the temperature dependence. To explain our model the easiest way is to give an example.

Let us suppose that we have the following reaction:

$$aA + bB \overset{v}{\rightarrow} C + D \tag{10}$$

We are interested only in the reaction from left to right. Then in our model, the velocity v is equal to:

$$v = k * [A]_t^a * [B]_t^b \tag{11}$$

where k is a constant and $[A]_t$ means concentration of A ($\frac{N_A(t)}{V}$) and the t subscript is there to remind us about the time dependence of the concentration.

So for our reactions, we get:

1. $v_1(t) = k_1[H]_t^2$ and $v_{-1}(t) = k_{-1}[D]_t$

2. $v_2(t) = k_2[D]_t[H]_t$ and $v_{-2}(t) = k_{-2}[^3He]_t$

3. $v_3(t) = k_3[^3He]_t^2$ and $v_{-3}(t) = k_{-3}[^4He]_t[H]_t^2$

2.3.2 The advanced model for the velocity

For the second model, k is no more a constant and it depends on the temperature. For an exothermic reaction

$$k(T(t)) = k(T_c) \times e^{(1-\frac{T(t)}{T_c})}. \tag{12}$$

And for an endothermic reaction:

$$k(T(t)) = k(T_c) \times e^{(\frac{T(t)}{T_c}-1)}. \tag{13}$$

$T(t)$ is the temperature and T_c the temperature for which we now the value of $k(T_c)$. You can link the temperature to the energy per particle by using the Boltzmann constant (8).

So we get for our velocities:

1. $v_1(t) = k_1(T_c)[H]_t^2 \times e^{(1-\frac{T(t)}{T_c})}$ and $v_{-1}(t) = k_{-1}[D]_t \times e^{(\frac{T(t)}{T_c}-1)}$

2. $v_2(t) = k_2(T_c)[D]_t[H]_t \times e^{(1-\frac{T(t)}{T_c})}$ and $v_{-2}(t) = k_{-2}[^3He]_t \times e^{(\frac{T(t)}{T_c}-1)}$

3. $v_3(t) = k_3(T_c)[^3He]_t^2 \times e^{(1-\frac{T(t)}{T_c})}$ and $v_{-3}(t) = k_{-3}[^4He]_t[H]_t^2 \times e^{(\frac{T(t)}{T_c}-1)}$

In this model, the reaction velocity will be influenced by the energy density of the star.

3 The code

3.1 Introduction

The goal of the code to be implemented is to solve numerically the coupled equations seen in the previous section in order to study their solutions and the properties of the simulated star (Temperature, energy radiated, life time, ...). The program should be able to:

1. Read a file of parameters and physical values.

2. Solve the basic model using Euler method.

3. Solve the other model using Euler and Midpoint method

Moreover a gnuplot script should be written to plot the results.

3.2 Inputs values and lecture of a parameter file

As all simulation programs: you have two kind of inputs: physical inputs and numerical inputs. The physical entries correspond to the values of your physical quantities that are necessary to solve the equations. In our case they correspond to:

1. initial concentration of all the nuclei

2. initial energy

3. volume of the star

4. value of k or value of $k(T_c)$

5. value of T_c.

Moreover, the program needs extra parameters (numerical inputs) to work. In our case this is:

1. the step-size for the time

2. the different options.

In order to make an user friendly program: it should read the data from a file in which the user has only to give the value of the parameters.

To write such function, I suggest you to use "`scanf`" to look for a specific chain of characters that is just before the value. Then using once again "`scanf`" to read the value. An example of parameter file is given at the end.

In this example, to read the value of the volume, you just have to look for "`Volume_of_star_in_km^3`" and you know that the next thing you read is the value $1.412e + 18$.

3.3 C function to solve equations

The C function to solve equations has to be written with two methods: Euler method and Midpoint method (Runge-Kutta 2nd order). There is some excellent Wikipedia articles on those two methods[1], please refer to them. Concerning your program, the user should be able to choose between the basic model or the advanced one. For the basic model, the user should be allowed to choose between the Euler method and the Midpoint method.

You also have to provide a way to stop the program if the solution become unphysical (negative energy, negative concentration of nucleus, ...).

All our functions to solve equations should have as imputs:

1. The values of the different k

2. The initial values of the concentrations of nuclei

3. The initial value of the energy

4. The surface value

5. The step size value.

6. For the advance model: the critical temperature.

example:

```
void midpoint_resolution_ad(double k[], double Initial_Concentration[], double Initial_E, double S,
double step_size, double Tc);
```

3.4 Results and gnuplot script

It should exist in your program a printing function. The printing function is a simple function which will print the results in a way that it could be used directly in gnuplot. The external gnuplot script should plot directly the quantity of interest in 4 plots:

1. Hydrogen concentration

2. All the others concentrations

3. The energy emitted

4. The temperature

---

[1]http://en.wikipedia.org/wiki/Euler_method, http://en.wikipedia.org/wiki/Midpoint_method

As example, your result file could looks like:

```
# Result for Euler Method
#
# t  [H]      [D]      [3He]    [4He]    dE       Energy    T
0 1.000000 0.000000 0.000000 0.000000 0.000000 0.000000 0.001792
1 0.999800 0.000100 0.000000 0.000000 0.000150 0.000010 0.001891
```

An example of plot is given at the end.

3.5   Difficulties

The main difficulties in the project are not really the programing of the algorithm but they are more related to deal with physical values. Here you will be confronted with huge numbers as the size of the star, its energy or the age of the star but also really small numbers as the velocity of the reaction. This kind of problems appears quite often in numerics and you should find an intelligent way to solve it.

3.6   Numerical values

Most of the numerical values can be found on Wikipedia. The ones which are missing are the values for the different k. You can play with those values, to see the impact of those factors on our model. Nevertheless to have an idea of the physical value of those parameters, here is some example:

$$
\begin{aligned}
k_1 &= k_1(T_c) = 9.8 \times 10^{-10} \mathring{A}^3.ky^{-1} \\
k_2 &= k_2(T_c) = 1.5 \times 10^{-4} \mathring{A}^3.ky^{-1} \\
k_3 &= k_3(T_c) = 1.1 \times 10^{-6} \mathring{A}^3.ky^{-1} \\
k_{-1} &= k_{-1}(T_c) = k_1 \times e^{(-E_1)} ky^{-1} \\
k_{-2} &= k_{-2}(T_c) = k_2 \times e^{(-E_2)} ky^{-1} \\
k_{-3} &= k_{-3}(T_c) = k_3 \times e^{(-E_3)} \mathring{A}^6.ky^{-1}
\end{aligned}
\tag{14}
$$

where $\mathring{A}$ is an angstrom and ky is for kiloyears (10^3 years). And T_c the critical temperature is:

$$
T_c = 3.10^6 K
\tag{15}
$$

3.7   Example of parameter file

YOUR FILE:

Physical_Value:
=========

Volume_of_star_in_km^3
$1.412e+18$

Initiate_concentration_in_angstrom^3
Hydrogen
1.0e+00
Deuterium
00e+00
Helium_3
00e+00
Helium_4
00e+00

Initiate_energy_in_Mev

00e+00

Critical_temperature
1.0e+07

Values_of_k
k1_in_angstrom^3_kiloyears^-1
$9.8e-10$
k2_in_angstrom^3_kiloyears^-1
$1.5e-5$
k3_in_angstrom^3_kiloyears^-1
$1.1e-6$
k-1_in_angstrom^3_kiloyears^-1
$2.3e-11$
k-2_in_angstrom^3_kiloyears^-1
$6.2e-08$
k-3_in_angstrom^3_kiloyears^-1
$2.9e-12$

Options:
=====

option_method_(Euler=0_Midpoint=1)
0

option_model_(Basic=0_Advanced=1)
0

Numerical_parameter:
===========

step_size_in_years
1000

3.8   Example of plot

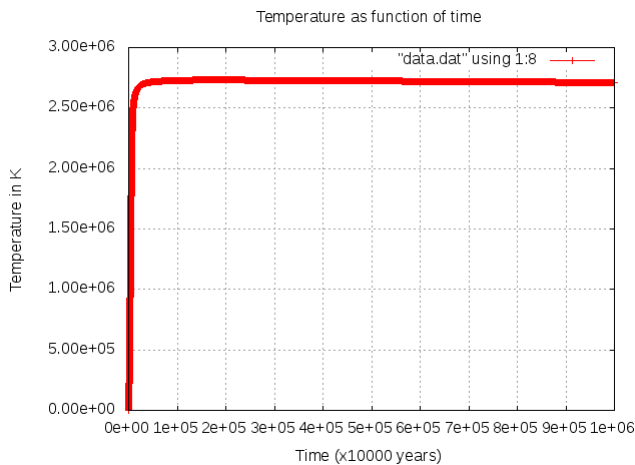For these plots the parameters used are those given by the example of parameter file.

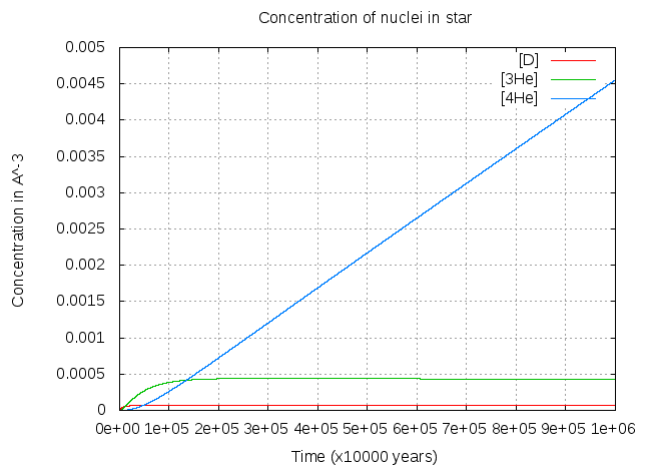Figure 1: Graphic of the temperature of the simulated star

Figure 2: Graphic of the concentration of Deuterium, Helium 3 and Helium 4 of the simulated star

6