Summer Research Scholarship 2004/2005
Final Report

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1 Project Description

This project has focused heavily on a paper given to me by my Supervisor, Dayal T. Wickramasinghe, entitled **Time Dependent Non-LTE Calculations of Ionisation**. Written by R. Wehrse, himself, and R. Davé, the paper describes a new numerical method for solving a particular pair of coupled partial differential equations. The paper also presents the results obtained from solving these equations with various initial/boundary conditions, and the project involved writing a Fortran code to reproduce the results shown in the paper, with some possible extensions should time permit.

2 Some Background

The Universe today is mostly made up of ionised hydrogen atoms. It is known that at the time of recombination, when the universe became transparent to electromagnetic radiation and the Cosmic Microwave Background was emitted, that the dominant matter in the universe was neutral hydrogen. At some time between the epoc of recombination and today, most probably when the first stars began to shine, the bulk of the universe became ionised. This 'epoc of reionisation' is the subject on much research.

Now, suppose we have a young star immersed in a field of neutral hydrogen. When this star begins to shine, the radiation it emits will ionise the surrounding gas according to the equations described below, and it is this ionisation that we model.

3 The Equations

The rate of ionisation at any given point is governed by two things:

1. The amount of incoming radiation at that point
2. The amount of already ionised hydrogen (and hence the number of free electrons) at that point

Also, the rate at which radiation propagates at a point is dependent on the amount of neutral hydrogen, as well as the Source function (which describes how the gas itself radiates, and for our purposes may be set to zero).

So, the two coupled partial differential equations to be considered are:

The Radiative Transfer Equation

$$\frac{\partial I(x,t)}{\partial x}\frac{\partial I(x,t)}{\partial x} = -\sigma N_0(x,t)(I(x,t) - S(x,t)) \tag{1}$$

and the rate equation for the number density of neutral hydrogen atoms

$$\frac{\partial N_0(x,t)}{\partial t} = -\sigma J N_0(x,t) + \alpha(N_{tot} - N_0(x,t))^2 \tag{2}$$

Where:

- σ = Photoionisation cross-section
- α = Recombination coefficient
- J = Mean intensity of the radiation field
- I = Local radiation intensity
- N_0 = Number density of neutral hydrogen atoms
- N_{tot} = Total hydrogen number density
- S = Source function. This is set to zero, and is ignored henceforth

These equations are subject to the initial conditions $N_0(x,0) = N_{tot}$ and the boundary condition $I(0,t) = I_{irr}$ where I_{irr} is the (specified) intensity of the ionising source. Thus, when the star begins to shine, the surrounding hydrogen is completely neutral.

4 The Method

Equations (1) and (2) cannot be solved analytically, so a numerical scheme must be undertaken. If we note that light rays propagate always in the same direction, then the specific intensity at x^{i+1} depends only on the specific intensity at x^i, and the absorption coefficients in $dx = x^i \ldots x^{i+1}$.

We can discretise the equations as follows:

$$\begin{aligned}\frac{N_0(x^{i+1},t^{k+1}) - N_0(x^{i+1},t^k)}{t^{k+1}-t^k} &= -\sigma N_0(x^{i+1},t^{k+1}) I(x^{i+1},t^{k+1}) \\ &\quad + \alpha\left(N_{tot}(x^{i+1}) - N_0(x^{i+1},t^{k+1})\right)^2 \end{aligned}\tag{3}$$

and

$$\frac{I(x^{i+1},t^{k+1}) - I(x^i,t^{k+1})}{x^{i+1}-x^i} = -\sigma N_0(x^{i+1},t^{k+1}) I(x^{i+1},t^{k+1}) \tag{4}$$

If we solve equation (3) for $I(x^{i+1}, t^{k+1})$, we can insert this into equation (4) to get

$$\frac{N_0(x^{i+1}, t^{k+1}) - N_0(x^{i+1}, t^k)}{t^{k+1} - t^k} = \frac{-\sigma N_0(x^{i+1}, t^{k+1}) I(x^i, t^{k+1})}{1 + \sigma N_0(x^{i+1}, t^{k+1})} + \alpha \left(N_{tot} - N_0(x^{i+1}, t^{k+1})\right)^2 \tag{5}$$

Now, if $I(x^i, t^{k+1})$ is known, then equation 5 reduces to a cubic in one variable, namely $N_0(x^{i+1}, t^{k+1})$, which can easily be solved numerically. Thus, we can move across the $x - t$ plane using the value of N_0 from the previous timestep, and the I from the previous position-step to solve for the current value of N_0, and then update I using equation (3)

5 The Results

A FORTRAN code was written to implement the above algorithm in one dimension, and after much tinkering, the results from the paper were reproduced (at least qualitatively).

Two other numerical algorithms were developed. One to deal with a radiation source at both ends of the computational grid, with the intention of generalising the method to allow for multiple sources. The other was to include a term in equation (1) that has been considered negligible (the left hand side should read $\frac{1}{c}\frac{\partial I(x,t)}{\partial x} + \frac{\partial I(x,t)}{\partial x}$).

However, neither of these were implemented, due to time constraints.