

Current Development of the Photo-Ionization Code Cloudy

P.A.M. van Hoof^{1,2}, P.G. Martin¹, G.J. Ferland²

¹*Canadian Institute for Theoretical Astrophysics, University of Toronto, McLennan Labs, 60 St. George Street, Toronto, ON M5S 3H8, Canada*

²*University of Kentucky, Department of Physics & Astronomy, 177 CP Building, Lexington, KY 40506-0055, USA*

Abstract. This paper describes the development of the photo-ionization code Cloudy since the last major release 90.05.

1. Introduction

This poster centers on the development of Cloudy, a large-scale code designed to compute the spectrum of gas in photo-ionization or collisional balance. Such plasma is far from equilibrium, and its conditions are set by the balance of a host of micro-physical processes. The development of Cloudy is a three-pronged effort requiring advances in the underlying atomic data base, the numerical and computational methods used in the simulation, and culminating in the application to astronomical problems. These three steps are strongly interwoven.

In recent years, Cloudy has undergone a major upgrade in the atomic data. A large part of this effort was concentrated on improving the photo-ionization cross sections. Since then the code has been transformed from a Fortran 77 to an ANSI C code and work has begun to completely recode the model atoms used to calculate line emissivities. They will be organized in such a way that each iso-electronic sequence has a common code appropriate for all members of that sequence. This makes validating the code easier and also facilitates future upgrades in the atomic data. Work on the hydrogen sequence is complete and work on the helium sequence is underway. A more detailed account of the current status of the code can be found in Section 2. The grain model in Cloudy is also currently undergoing a major upgrade, which is described in more detail in Section 3.

2. Improvements in Cloudy 94

Cloudy has undergone a major transformation in the past year with respect to the last release Cloudy 90. The most important differences are listed below. A first release of Cloudy 94 is currently available from the Cloudy web-site (for details see Section 4).

- The code is now strict ANSI/ISO 89 C. As a result Cloudy is now exceptionally GNU gcc and Linux friendly. After this version is released the

development version will move to C++ as gcc evolves onto the ANSI/ISO C++ standard and the C++ standard template library matures.

- All hydrogenic species H I through Zn XXX, and their respective ions are treated with a common model atom that uses a single code base. This atom reproduces accurate hydrogenic emissivity to within the uncertainties in the atomic data. The 30 hydrogenic ions can have up to 400 levels.
- The continuum now extends down to 10^{-8} Ryd ($\lambda \approx 10$ m). This is needed because the continuum must extend to the energy of the 400 – 399 transition of hydrogen.
- Previous versions used simple approximations for the hydrogenic ionization and level balance for temperatures too low to compute NLTE departure coefficients. The new version determines level populations for low temperatures rather than departure coefficients, so low temperature predictions are as valid as high temperature results.
- Two additional sets of NLTE stellar atmospheres are available – the CoStar grid of wind-blanketed O-stars, and the Rauch low-metallicity grid of white dwarf atmospheres.
- The optimization algorithm PHYMIR is included. This allows optimization runs to be executed much more efficiently on parallel UNIX computers by calculating individual models simultaneously on different processors. This can drastically reduce the amount of wallclock time needed, depending on the number of free parameters.
- The ionization/thermal kernel has been totally rewritten to incorporate all the lessons learned from known convergence problems. As a result C94 is more stable than C90, with far better convergence properties.
- All previous versions only considered ionization stages that could be produced by the incident continuum. This limit has been lifted, so collisional or coronal equilibrium models can be computed with very soft incident continua.
- Much of the code is now double precision. As a result the code will work for a broader range of densities than before. Densities well below 10^{-5} cm $^{-3}$ or above 10^{17} cm $^{-3}$ can be computed without under/over flow.
- The assert command has been introduced. This tells the code to verify that its predictions agree (within a stated uncertainty) with a known result. The test cases make extensive use of this feature, which provides an automatic way to validate the code. As of now, the entire test suite of standard models is recomputed and verified every single night.
- All large storage items are dynamically allocated at run time, taking only the needed memory. As a result, in its default state, C94 actually takes less memory than C90. It also executes slightly faster than C90.

Figure 1. The absorption cross section for astronomical silicate for three single sized grains. The dust-to-gas ratio is the same for all three species and the cross sections are normalized per hydrogen nucleus in the plasma.

3. The Grain Model

The current grain model was introduced to Cloudy in 1990 to facilitate more accurate modeling of the Orion nebula (for a detailed description see Baldwin et al., 1991, ApJ 374, 580). The model has since undergone some minor revisions but remained largely the same. Recently, our knowledge of grains has been greatly advanced by the results from the ISO mission. In view of these rapid developments we have undertaken a major upgrade of the grain model in Cloudy. The two main aims are to make the code more flexible and to make the modeling results more realistic.

In particular, in the current model the grain opacities for a handful of grain species are hard-wired in the code. Furthermore, only a single equilibrium temperature is calculated for each species. This is inappropriate for a grain size distribution since small grains will be hotter than large grains. This is caused by the fact that grain opacities depend quite strongly on grain size, as shown in Figure 1. To improve the model, the following changes are being implemented:

- We will include a spherical Mie code in Cloudy. The necessary optical constants needed to run the code will be read from a separate file. This allows greater freedom in the choice of grain species. Files with optical

constants for a range of materials will be included in the Cloudy distribution. However, the user can also supply his own optical constants for a completely new grain type.

- We will introduce mixing laws to the code. This will allow the user to define grains which are mixtures of different materials. Cloudy will then calculate the appropriate opacities by combining the optical constants of these grain types. This will allow the user to simulate aggregate or ‘fluffy’ grains.
- The absorption and scattering opacities will be calculated by Cloudy for more arbitrary grain size distributions. This will give the user considerably more freedom. Currently only a standard ISM and a truncated Orion size distribution are included in the code.
- The size distribution will be split up in many small bins, and an equilibrium temperature will be calculated for each bin separately. This allows non-equilibrium heating to be treated and more realistic grain emission spectra to be calculated. First tests show that under realistic conditions this can make large differences in the flux (at least a factor of two) in the Wien tail of the grain emission. The total flux emitted by the grains remains virtually unchanged however.

4. Cloudy on the Web

The source for Cloudy can be obtained from the web at the following URL:

<http://www.pa.uky.edu/~gary/cloudy>

This site contains the current major release (Cloudy 90.05) as well as the beta2 release of Cloudy 94 (actually called Cloudy 93.03).

You can add your name to the Cloudy mailing list by logging on to the following URL:

<http://nimbus.pa.uky.edu/cloudy/versions.htm>