INTRODUCTION

Physical conditions in nebulae (planetary nebulae, large HII regions) are usually obtained using so called diagnostic method, that allows to obtain average the electron temperature T_e and density N_e from different emission line intensities ratios (see, f.e., DIAGN method [1]). However, in case of diagnostic methods obtained T_e and N_e are constant within investigated ionization zone. For detailed analysis of the ionization structure of nebular environment the transfer of the ionizing radiation taking into account all elementary processes in nebular plasmas important for such transfer should be calculated. Such calculations are performed during PhM of nebular environment.

In case of nebulae with compact ionization source (f.e star, compact stars cluster, etc) radiation can be separated into two components:

1. Direct component, comming from ionizing source;
2. Diffuse component, originating from nebular gas.

While transfer of the direct component of the ionizing radiation can be easy calculated (because of no source terms), the diffuse radiation transfer calculation is a very time consuming even for modern supercomputers, since it requires iterative process of ionizing radiation flux integration over volume in each elementary cell of nebula environment. For time economy purpouses approximate methods of diffuse radiation calculation are frequently used. The most popular are QTS approximation, that assumes that ionizing radiation is consumed into the same volume where it whas emited, and Qutward Only approximation, that assumes that ionizing radiation is propogated in radial direction, from ionizing source to outer surface of object. However, OTS method is good only in case of optically thick objects. Outward only approximation is more precise, however it can be inacurate in case of objects with complicated morphology. For example, dense clumps can cause the origination of shaded regions behind of them. Non-radial DIR can play main role in formation of the ionization structure in these shaded regions.

To avoid usage of approximate methods for DIR calculation and reduce time, required for PhM we developed DiffRay3D) software, that allows to integrate radiation fluxes using 2D or 3D emissivity maps, and, as result, to implement method for detailed diffuse radiation calculation, described in [2] and displayed in Figure 1.

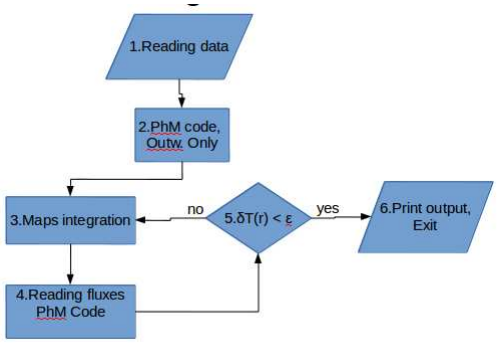

Figure 1: Our approach algorithm

1 - Reading data, such as required precision, maximum iterations, etc.

2 - Running PhM code in Outward Only mode, generating and saving emissivity and opacity maps.

3 - Running integration procedure using previously generated maps.

4 - Running PhM code, using fluxes, obtained after step 3. Generating and saving new emissivity and opacity maps.

5 - Check difference between electron temperatures obtained from current iteration and the previous one. Once difference is greater than is required by precision, pointed in 1, then returning to step 3.

6 - Printing fluxes and ionization structure, obtained from PhM on last iteration.

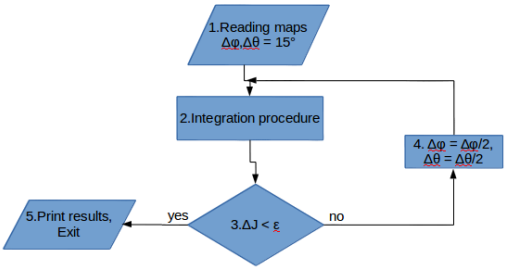

Figure 2: DiffRay algorithm

1 DiffRay3D. General algorithm and limitations

Current DiffRay3D version provides tools for radiation fluxes integration using 2D maps over 3D volume (3D maps support will be implemented in next code versions). Nebula is divided onto 80 sectors (20 per quoter, assuming cylinder symethry and physical conditions in each quoter are the same). Each sector divided onto slabs. Shell structure is defined from input emissivity/opacity maps.

General code algorithm is displayed below:

For diffuse radiation fluxes integration procedure implementation DiffRay code was developed. The algorithm of code is given on figure 2.

1 - Setting up initial integration steps for angles, reading emissivity and opacity maps, that should be integrated.

2 - Integration of diffuse radiation fluxes for each elementary volume of nebula environment

3 - Comparing if difference between fluxes, obtained on current iteration and previous one. If it fits required precision, exit to 5. Elsewise, decreasing integration step (4), and returning to 2.

5 - Print fluxes in format, that can be readen by PhM code. Exit.

2 How to launch code

To run code, you need working compiled code version, and valid object data with commands file provided.

2.1 Code compilation

1. Download code archive.
2. Unzip files in any folder you wish. DiffRay3D can be started into any folder, the only demand is code should have enough permissions for create/delete folders and files.
3. Once unzipped, go to "source/v*.*.*/" folder, and run MakeFile.all. This should create DiffRay3D.exe executable into instalation root folder.

2.2 Input data format

To work correctly, code should have information about objects geometry, emissivity and opacity maps, so on. This information is readen from data folder. In general, filename looks like:

Emis_Lines_SectorNo**Sector number**_Age**Object age**Myr.dat

Here Sector number is number of represented by file sector Age can be used as any identifier for model data set. (F.E. once you have maps for several models, you can enumarate them, and use this numeration in age field.

Complete list of supported data files:

Continuum1_Last_Age10.00Myr.dat - file with continuum energy mesh structure. Each row should contain into first column continuum cell energy in Rydbergs. File is required.

Emis_Cont_SectorNo1_Age10.00Myr.dat - file with continuum emissivity data. Each row corresponds to sector slab. First row has only one value - inner radius. Next rows contain slab outer radius in first column, and emissivity values for each energy cell in following columns. File is required.

Opac_Cont_SectorNo1_Age10.00Myr.dat - file with opacity data for each continuum cell. Each row corresponds to sector slab. First row has only one value - inner radius. Next rows contain slab outer radius in first column, and opacity values for each energy cell in following columns. Used both for continuum and lines optical depth calculation. File is required.

Emis_Lines_SectorNo1_Age10.00Myr.dat - file with lines emissivity data. Each row corresponds to sector slab. First 2 rows has heading, according to standart Cloudy "punch line emisivity" command, [3]. Next rows contain slab outer radius in first column, and emissivity values for each emission line in following columns. File is required.

Abund1_Age10.00Myr.dat - file with elemental aundances data. Each row corresponds to sector slab. First row should have valid column headings with element names, provided as first 4 symbols of full name. (#Depth H HELI LITH BERY..., Garry Ferlands Cloudy output format, see [3]). Next rows contain slab outer radius in first column, and elemental abundances for each element in following columns. File is not required.

2.3 commands.ini file

Once you have compiled code and prepared data files, you should write some instructions for how and what code should calculated. These instructions are contained into commands.ini file into instalation root directory.

An example is distributed with code source.

IO settings

print directory "path to your output folder, relative to instalation root directory"
input directory "path to input data files folder, relative to instalation root directory"

Example:

print directory result/ngc/ism0/140
input directory data/ngc1569nograin
Please, note that paths should be provided without quotes!

Distance

distance log10_dist units.

Example:

distance 19.87 km
(Distance to object is adopted of $10^{19.87}$ kilometers. Supported units are meters, kilometers, centimeters.

Object

phi x , x - objects azimuthal rotation angle relating to observer sight ray in radians;
theta x , x - objects vertical rotation angle relating to observer sight ray in radians;
age x, x - object age, or another models bundle identifier;

Example:

object phi 0.76
object theta 0.21
object age 50

Integration

maxiterations x, x - maximum code iterations. This option is useful to prevent code falling into endless loop when trying to converge.
precision x, x - acceptable convergence between iterations, 0.01 - 1%. mode outw - switches code to Outward Only mode, is good thing for tests.

Example:

integration precision 0.005

integration maxiterations 12

Aperture

aperture phi theta w h - Adds aperture to list of apertures to be calculated. Here phi - azimuthal aperture position, theta - vertical position relative to ray from observer to center of object. w, h - aperture width and height. All values should be provided into radians.

Example:
apperture add 0 0 0.000014537 0.000014537
apperture add 0.000464 0.0000139 0.000014537 0.000014537
apperture add -0.000271 -0.0000102 0.000014537 0.000014537
In this example code will run calculations for 3 apertures, and put results to app{N} folder. N is aperture number here. Aperture folders are created automatically into directory, specified with output command.

References

[1] Golovaty V. V., Dmiterko V. I., Mal'kov Yu. F., & Rokach O. V. 1993, Astronomical Report, Vol. 37, Issue 4, pp. 346-354

[2] O. S. Buhajenko, B. Ya. Melekh 2016, 'METHOD FOR DETAILED CALCULATION OF THE DIFFUSE IONIZING RADIATION IN NEBULAR ENVIRONMENTS', Ivan Franko National University of Lviv, 4901 (13 p.)

[3] Ferland G.J. 1999, 'Hazy, a Brief Introduction to Cloudy 94', University of Kentucky, Physics Department Internal Report; `http://www.nublado.org`