### ABSTRACT OF DISSERTATION

Dejan Vinković

The Graduate School

University of Kentucky

2003

#### 2D RADIATIVE TRANSFER IN ASTROPHYSICAL DUSTY ENVIRONMENTS

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A dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the College of Arts and Sciences at the University of Kentucky

By

Dejan Vinković

Lexington, Kentucky

Director: Prof. Moshe Elitzur, Professor of Physics and Astronomy

Lexington, Kentucky

2003

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#### ABSTRACT OF DISSERTATION

### 2D RADIATIVE TRANSFER IN ASTROPHYSICAL DUSTY ENVIRONMENTS

I have developed a new general-purpose deterministic 2D radiative transfer code for astrophysical dusty environments named LELUYA (*www.leluya.org*). It can provide the solution to an arbitrary axially symmetric multi-grain dust distribution around an arbitrary heating source. By employing a new numerical method, the implemented algorithm automatically traces the dust density and optical depth gradients, creating the optimal unstructured triangular grid. The radiative transfer equation includes dust scattering, absorption and emission. Unique to LELUYA is also its ability to self-consistently reshape the sublimation/condensation dust cavity around the source to accommodate for the anisotropic diffuse radiation.

LELUYA's capabilities are demonstrated in the study of the asymptotic giant branch (AGB) star IRC+10011. The stellar winds emanating from AGB stars are mostly spherically symmetric, but they evolve into largely asymmetric planetary nebulae during later evolutionary phases. The initiation of this symmetry breaking process is still unexplained. IRC+10011 represents a rare example of a clearly visible asymmetry in high-resolution near-infrared images of the circumstellar dusty AGB wind. LELUYA shows that this asymmetry is produced by two bipolar cones with  $1/r^{0.5}$  density profile, imbedded in the standard  $1/r^2$  dusty wind profile. The cones are still breaking though the  $1/r^2$  wind, suggesting they are driven by bipolar jets. They are about 200 years old, thus a very recent episode in the final phase of AGB evolution before turning into a proto-planetary nebula, where the jets finally break out from the confining spherical wind. IRC+10011 provides the earliest example of this symmetry breaking thus far.

**KEYWORDS**: Radiative Transfer, Circumstellar Dust, AGB stars, IRC+10011, Theoretical Imaging

> Dejan Vinković (Author's Name) Sep 22, 2003

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### 2D RADIATIVE TRANSFER IN ASTROPHYSICAL DUSTY ENVIRONMENTS

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To my late Mother.

#### ACKNOWLEDGMENTS

Homer Simpson, one of the most "influential philosophers" of our times, says: "*Trying* is the first step towards failure". These words of "wisdom" were tormenting me five years ago when my PhD adviser, Moshe Elitzur, proposed developing a two-dimensional radiative transfer code as the topic of my dissertation research. His idea of the basic numerical algorithm that I should implement in the code consisted of some hand-waving, and the sentence: "Take this 1D stuff and then do something with it...". I knew then that I was facing a big project and an even bigger risk of failing even after many years of work. Homer Simpson, in his infinite wisdom also says: "Stupid risks make life worth living." This is precisely what happened with my project!

I am greatly indebted to Moshe for believing in me and encouraging me to work on this project. I am also appreciative of his guidance, his insights, and well-founded criticisms. His tolerance for my temper, and his willingness to allow me to express my creativity through my own projects and endeavors unrelated to my PhD research will always be with me.

In addition, special thanks are due to Željko Ivezić for his support, encouragement and advice. I would not achieve even close to what I did if it was not for him.

The work described in the last chapter of this dissertation was a collaboration with the Infrared Interferometry Group at the Max-Planck-Institut für Radioastronomie, Bonn, Germany. Special thanks go to Gerd Weigelt, the director of the group, for his support and hospitality during my multiple visits to the Institute.

If you flip through the pages of this dissertation, you will often see the name Leluya. This is not only the name of my computer code that this dissertation is based on, but also the name of a pre-Christian Croatian goddess of lightning. It was Lidija Bajuk Pecotić who proposed this name and provided the beautiful mythical stories behind it. Marko Čavka provided a touch of his design talent by making a cool logo, web-pages for Leluya (www.leluya.org), and a design for my conference posters. I thank them both because without their help Leluya would not have the appeal it has.

What you can not see from my dissertation is that I have been involved in several other

research projects. I would like to thank Anatloy Miroshnichenko for his longstanding collaboration in the project about young stellar objects.

There is also research on meteors, which has a very special place in my heart. For that I am grateful to the "Mongolia team": a group of my good, old friends who put together an expedition to Mongolia in 1998 to study sounds from meteors. They accepted me as a team member and we ended up in an adventure that has taken us a long way since those freezing nights of mid November of 1998 in the Mongolian wilderness. I am extremely grateful to the expedition team leader Slaven Garaj for his friendship and guidance of that project. I also thank Pey-Lian Lim , who joined me on this project later on. Thanks to Stipe Klarich, Pey-Lian and I had antennas to work with, and thanks to Teresa Moody, we "explored" eastern Kentucky while testing our equipment. Also, thanks to Bruce Gillespie we enjoyed the hospitality of the Apache Point Observatory while observing meteors in November 2002. I am also thankful to Teresa for correcting my English in many occasions.

Speaking of correcting my English, there is nobody who "suffered" more than Helen Klarich. Well, maybe Robert Bauman because of his very studious and time consuming approach to this job. I thank them both. And I thank them for their friendship that has made my life here in Lexington enjoyable, together with friends like Ninfa Floyd and Jordi Moya-Larano, to name a few.

Of course, those who helped me the most with my life here in Lexington are Ivica Reš and Ivana Mihalek . Lets be honest: they adopted me while they lived here. What can I say ... thanks guys!

I also thank my colleagues and friends in znanost.org, a non-profit organization promoting the public understanding of science. We know that we are going to change the world ... yeah, right! It is worth trying, though, and it is their work and enthusiasm that keeps that dream alive in me.

Last, but not least, I want to thank my family for their love and support: my dad Ivan Vinković, my brother Mladen Vinković and his wife Dijana Matak Vinković.

All in all, I can say that I have been blessed with having so many friends. They have shaped my life and they continue to do so. People like Igor Gašparić with his sense of humor, and people like Korado Korlević with his view of life. Thank you all!

Moshe often likes to say that he has "aged." Thus, I would like to remind him of what Homer Simpson has to say about old people: "...old people don't need companionship. They need to be isolated and studied so it can be determined what nutrients they have that might be extracted for our personal use".

.... D'oh!!

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 $1.7 \mathrm{Mb}$ 

# Chapter 1 Introduction

In its most general description, radiative transfer deals with the transport of radiation through a medium. Radiation can be absorbed, scattered, or emitted by the medium. The same formalism used for describing this transport can be applied to the transport of neutral particles, such as neutrons (e.g. Carlson 1963) in the core of a nuclear reactor or photons scattered through the human head as in the optical tomography (e.g. Boas and Gaudette 2001). Astrophysics is especially dependent on the understanding of radiative transfer. Applications range from the theories of stellar interiors, stellar atmospheres, planetary atmospheres, circumstellar and interstellar clouds, galaxies, all the way to the cosmological models.

Although the radiative transfer equations look simple at the first sight, they represent a numerically challenging and multidisciplinary problem. Subrahmanyan Chandrasekhar, who made many breakthroughs in this field of work during the 1950's, once said (Cropper 2001):

My research on radiative transfer gave me the most satisfaction. I worked on it for five years, and the subject, I felt, developed on its own initiative and momentum. Problems arose one by one, each more complex and difficult than the previous one, and they were solved. The whole subject attained an elegance and beauty which I do not find to the same degree in any of my other work.

The research described in this dissertation is focused on the spectral continuum of a dust cloud around or nearby a heating source, such as a star or a galactic nucleus. This represents a basic astrophysical problem and its solution is highly needed by the astronomical community. In order to explain a vast number of observed astronomical phenomena, astronomers increasingly seek an accurate solution to the radiative transfer and dust temperature distribution. Unfortunately, there is a lack of multidimensional codes that can keep up with the increasing requirements for more detailed and precise theoretical modeling. An additional problem is a lack of diversity of multidimensional algorithms, considering that the Monte Carlo method is used in currently the best codes and, thus, their precision can not be independently tested.

Encouraged by the success of the 1D code DUSTY developed by Ivezić, Nenkova, and Elitzur (1999), in 1998 our research group embarked on a development of a code for an axially symmetric two dimensional dust distribution. The goal was to have a code without any limits on its resolution and 2D geometry, though it became apparent quite soon that this is an extremely difficult task to achieve. One of the main reasons why multidimensional codes are not so advanced compared to the 1D codes is the way that they generate their computational grids. The realization that the algorithm for grid generation represents the heart of the problem led me to several years of code development. The outcomes are newly developed numerical algorithms and methods that go beyond the Monte Carlo method and provide the "exact solution" to the radiative transfer within this geometry. Nonetheless, these algorithms are not limited to the astrophysics of dust. They represent a completely new approach to the radiative transfer numerics.

As a result of this research, I have developed the code named LELUYA (*www.leluya.org*) where I implemented these new algorithms. LELUYA can automatically trace the dust density and optical depth gradients, creating the optimal adaptive grid. The grid is highly unstructured and triangular (i.e. grid cells are triangles without pre-defined constrains on their shape), a rarity among the radiative transfer codes. Different grids are created this way for different wavelengths to accommodate the spectral variation of dust opacity. The radiative transfer problem confined to the grid, including dust absorption, emission and scattering, is solved without approximations. The first preliminary results from LELUYA were obtained in spring 2002. They have been refined since then and evolved into the first scientific product of LELUYA, described in this dissertation.



Figure 1.1: Leluya - artwork by Lucia L. Klarich .

Design by Marko Čavka



LELUYA/LELIJA/LELUJA Goddess of lightning, weddings, and motherhood

LJELJUJA, PERUNIKA, SABLJA, SABLJARKA, STRIJELKA, IRIS

Author of the following ethnological description of the name LELUYA is **Lidija Bajuk Pecotić**:

Numerous and colorful (Iris is rainbow in Latin) meadow wildflower with saber-like leaves. Some species are widespread and very common, but some of them grow in very limited areas and have become endangered, e.g. Iris Croatica (Hrvatska Perunika, see picture) which grows only in the northern and northwestern Croatia. It grows in swampy sunny forest clearings. There are also exotic cultivated species that grow in parks and gardens.

This plant perunika got its name after the goddess of the sky Perunika (Perunka, Perunova, Perkunova, Perena, Gorka), wife of the old Slavic god Gromovnik (God of Thunder) Perun. This is also a name for a place hit by a Perun's spark (i.e. thunder, arrow, saber), or where a rainbow "touches" the ground.



Figure 1.2: Iris Croatica

A kajkavian (Croatian dialect) version of this name is Leluja (Ljeljuja), probably inflected form of Ljelja, which is another name of this goddess. It comes as no surprise, then, that people believed that carrying a dry root of perunika plant, if dug out on the Easter night, could protect from stings and strikes.

Perunika (later transformed into Veronika), i.e. Ognjena Marija (Fairy Mary), wears a rainbow as her belt. She is a goddess of lightning, weddings, and motherhood. Later, under Christianity, her importance was degraded and she was regarded as an evil goddess, described as an evil and ugly woman named Irudika, who was in turn a daughter of Poganica (exiled by Perun). Perunika punishes people with a heavy sledge. God of Thunder has thunder at his disposal (symbols of his sexual male potency), she has lightning at her disposal. The lightning comes in two so-called forms: elongated watery type and glassy type. The latter is ball lightning, a rare meteorological phenomenon, embodied during old times as apple, rosette, or female genital organ, in the mythical perception of the world. Thanks to Perunika's lightning, people learned about the fire and water in clouds.

For more information about the mythology of LELUYA follow the link: http://www.leluya.org/mythology.html

Concurrently with the development of LELUYA, I have worked on modeling the spectral energy distribution and theoretical imaging of massive pre-main-sequence stars (known as Herbig Ae/Be stars). For that purpose I used a hybrid 1D/2D version of DUSTY which implements an approximate model of a flat dense dusty disk imbedded in a tenuous halo (Miroshnichenko, Ivezić, Vinković, Elitzur 1999). The model yields numerous interesting theoretical insights into the evolution of the circumstellar environment of these stars. That work is not described in this dissertation, but the research goal is to eventually address those same problems with LELUYA.

### **1.1** Stochastic vs deterministic

Numerical radiative transfer methods are highly dependent on their field of application, as this allows implementation of specific simplifications. The common numerical difficulty, however, in all radiative transfer implementations is how to deal with the dimensionality of the system under consideration. The one-dimensional methods have been under development for almost a century. Very efficient algorithms have been developed in the last 40 years (Chandrasekhar 1960; for the latest review see Peraiah 2002). On the other hand, the multidimensional methods are not so advanced. The two-dimensional radiative transfer methods have gained some improvements in the 1990's, but they are still very limited in their applicability and essentially based on the decades-old methods. In general, multidimensional methods are mostly approximate in their radiative transfer physics or apply only to highly simplified geometrical structures (there is no general review of all the methods currently used in the context relevant to our research, but for a better insight follow the references within e.g. Steinacker et al. 2003, Wolf 2003, van Noort at al. 2002, Balsara 2001, Dullemond and Turolla 2000, Chick et al. 1996).

One method that bridges over all dimensions is the Monte Carlo technique. It has been quite a popular choice in all radiative transfer fields of study and a frontrunner in addressing more complex problems. Its popularity is largely driven by its simplicity and straight-forward logic. In a nutshell, the method works by following the evolution of a randomly emitted "particle" (that is, an "energy packet") until it exits the computational domain or gets destroyed. During this travel it goes through random interactions with the medium where it can lose some energy or change its direction of travel. After following a large number of such particles, we can collect enough statistics of particle-medium interactions to establish a balance between the locally absorbed and re-emitted energy in all parts of the computational domain.

Monte Carlo, however, suffers from a long list of problems that originate from the stochastic nature of the method. Many of those problems have been successfully addressed only recently (e.g. Wolf 2003, Bjorkman and Wood 2001, Gordon et al. 2001, Hogerheijde and van der Tak 2000, Lucy 1999). Nonetheless, not all of those "solutions" have spread to all Monte Carlo codes, probably because they make the whole approach and programming far more tedious.

Moreover, a few serious problems still remain. One of them is the error control. The only error associated with the quantities derived from Monte Carlo calculations (such as the dust temperature or the light intensity) is the statistical error. This error can be reduced only by use of an increased number of emitted particles. However, deterministic methods, like LELUYA, solve the equations on an underlying computational mesh. The mesh is a result of a discretisation procedure over the computational domain, which introduces systematic errors into the calculation. This is a useful feature because it allows a quantification of the computational error associated with a particular discretisation feature on the mesh. For example, we can quantify the influence of the local temperature or interpolation errors on the overall emerging light intensity. More importantly, deterministic methods allow us to detect and quantify a local deviation from the energy conservation and appropriately refine the associated computational grid.

This points out another serious problem of Monte Carlo: grid resolution. The statistics of the particle-medium interactions are derived on volume cells comprising a mesh. A problem arises when small spatial features need to be resolved. Since Monte Carlo methods trace the most likely events, the interaction probability is proportional to the cell's volume. Hence, it is difficult to "pump" enough particles into a small cell, especially if it is positioned far away from the central energy source. Introducing an artificial bias into the randomness of particle trajectories, in order to focus them toward a small cell to boost its statistics, is in collision with the basic principles of stochastic methods. Such a bias would create uncontrollable and unpredictable numerical errors. Deterministic methods do not have this problem because they solve the equations at the grid elements (vertices or cells). Therefore, Monte Carlo codes implement relatively simple grids that bear a tendency toward local uniformity, which imposes a priori limits on their application. In contrast, deterministic codes can use highly unstructured and non-uniform grids, as LELUYA does.

Unfortunately, there are drawbacks to the deterministic methods. They critically depend on the quality of the grid discretisation scheme. A too coarse grid creates fictitious energy sinks, while a too coarse angular grid mimics an energy source, both leading to large computational errors. Developing grid generation algorithms that can cope with these problems is a difficult and time consuming task. Consequently, the evolution of such algorithms has been slow. In the astrophysical context, LELUYA employs the most complicated radiative transfer grid known so far among the codes that can simultaneously handle the dust absorption, emission and scattering. Another problem with the deterministic methods is that they require considerable computational resources. This presses for the utilization of multiprocessor machines and development of efficient parallelization schemes. Hence, LELUYA employs a parallelization implementation with a newly developed scheme exploiting specifics of LELUYA's radiative transfer method. Fortunately, "supercomputers" are becoming an increasingly accessible commodity thanks to the increasing performance-over-price of Linux clusters.<sup>(1)</sup>

Finally, what should we use for multidimensional radiative transfer problems: deterministic methods or Monte Carlo? The answer depends intimately on the problem under considerations, including the quality of observational data. Before engaging into the "murky business" of radiative transfer modeling, we need to ask ourselves how much detail we want from the modeling. A large number of astrophysics problems can be addressed quite successfully by implementing various simplifications. Monte Carlo codes are ideal for tasks like that. There are problems, however, where such approaches have reached their theoretical limits. These are usually the most intriguing and still open problems in astrophysics.<sup>(2)</sup> They include, for example, the circumstellar dusty disk and halos around young pre-main-sequence (PMS) stars, the non-spherical dusty envelopes around AGB stars, and the clumpy dusty torus around the central source of the active galactic nuclei. For them we plan to use LELUYA for further investigations, as demonstrated in this dissertation on the problem of non-spherical circumstellar envelope of the AGB star IRC+10011.

### **1.2** Basics of dust extinction

The physics underlying radiative transfer is the interaction between electromagnetic radiation and a medium comprised of small particles, or "dust", as we call them. This dust alters the properties of a beam travelling through the medium. The basic quantity that describes the radiative transfer physics is the energy carried along by the beam. It is called specific intensity or brightness  $I_{\lambda}$  (or  $I_{\nu}$ ) and it describes how much energy  $dE_{\lambda}$  is passing through a unit area dA per unit time dt within a unit solid angle  $d\Omega$  per unit

<sup>&</sup>lt;sup>(1)</sup>As of August 2003, the performance record is \$84 per 1GFLOPS, achieved by the KAOS group at the University of Kentucky with their KASY0 Linux cluster (http://aggregate.org/KASY0).

<sup>&</sup>lt;sup>(2)</sup>Monte Carlo approach still does not have an alterative when polarization maps are considered. It is also the best choice for 3D geometries, since deterministic codes are very inaccurate and limited in their application (e.g. the 3D code described in Steinacker et al. 2003 has serious problems with the luminosity conservation in geometries with steep dust density gradients). In addition, Monte Carlo is still the preferred option in cases where anisotropic dust scattering is needed.

wavelength  $d\lambda$  (or frequency  $d\nu$ ):

$$dE_{\lambda} = I_{\lambda} \, dA \, dt \, d\Omega \, d\lambda \tag{1.1}$$

There are two extinction processes by which the dust reduces the intensity of a beam: absorption and scattering. Absorption converts absorbed photons into internal energy, which in turn increases the dust temperature, while scattering deflects photons from the beam. An extensive multidisciplinary science



Figure 1.3: Definition of intensity - see equation 1.1

is hidden behind those simple general definitions. The dust particles can be of various, often exotic shapes, structures and chemical compositions, with a range of sizes and electromagnetic properties. Similarly, the dust particles emit radiation by processes inverse to absorption. Thus, studying spectral changes caused by dust extinction and emission yields information about the observed astrophysical dusty environments. Due to the widespread presence of dust in the Universe, this astrophysical discipline has advanced in the last twenty years into one of the mainstream fields of study.

Even though the purpose of developing radiative transfer tools is to eventually investigate the dust properties around the Universe, this dissertation is focused on the study of radiative transfer processes once the dust properties are provided. What LELUYA needs is the dust optical properties in the form of absorption cross sections  $\sigma_{\lambda}^{abs}$  and scattering cross section  $\sigma_{\lambda}^{sca}$ , which combined give the extinction cross section:

$$\sigma_{\lambda}^{ext} = \sigma_{\lambda}^{abs} + \sigma_{\lambda}^{sca} \tag{1.2}$$

Cross sections represent the probability of interaction between an incident photon and a dust grain. It is a complicated function of the grain properties, photon wavelength and polarization, and the angle of outgoing photon relative to the incoming one. It is sometimes convenient to compare cross sections with geometric cross sections  $a^2\pi$ , where *a* is the dust grain's radius:

$$Q_{\lambda}^{ext,abs,sca} = \frac{\sigma_{\lambda}^{ext,abs,sca}}{\pi a^2} \tag{1.3}$$

 $Q_{\lambda}$  is called the efficiency factor.

In our investigations so far, we have used a simple model of spherical dust grains that radiate and scatter isotropically. This is, of course, a highly idealized description of real astrophysical dust particles, but reasonable enough as a starting point. Namely, real dust grains retain random orientations, which manifests itself as an averaged grain species similar to those of spheres. An additional convenience is that the absorption and scattering properties of spherical grains can be relatively easily calculated with the Lorentz-Mie theory. In Lorentz-Mie theory, the electromagnetic fields inside and outside the particle are derived from an infinite series of independent solutions to the wave equations, smoothly connected to each other by the boundary conditions on the particle surface. In this simplified picture, all we need from the solid state properties of the dust material is the complex refractive index<sup>(3)</sup>  $m_{\lambda} = n_{\lambda} - ik_{\lambda}$ . A pure dielectric, for example, has  $k_{\lambda} = 0$ and, therefore, no absorption. Astrophysical ices and silicates are examples of materials close to this limit with  $k_{\lambda} < 0.1$ . On the other hand, metals are examples of strong absorbers and their  $k_{\lambda}$  is of the same order as  $n_{\lambda}$ . An extensive review of the physics of astrophysical dust can be found in the recent book by Krügel (2003).

If we want to derive the total extinction produced by the dust then we need to know the dust number density  $N_d$ . In reality, however, grains of various sizes and chemistry are mixed together. Therefore, we specify a mixture of grain sizes where each grain type i has the number density  $n_i$ , such that  $N_d = \sum_i n_i$ , and the corresponding cross section  $\sigma_{\lambda_i}^{ext}$ . This finally leads to the extinction coefficient:

$$\kappa_{\lambda}^{ext} = \sum_{i} n_i \sigma_{\lambda,i}^{ext} = \sum_{i} \kappa_{\lambda,i}^{ext}$$
(1.4)

<sup>&</sup>lt;sup>(3)</sup>Quantities  $n_{\lambda}$  and  $k_{\lambda}$  are often called the *optical constants*, even though they are functions of wavelength. They are related to the dielectric permeability  $\varepsilon$  and the magnetic permeability  $\mu$  through the index  $m_{\lambda} = \sqrt{\varepsilon \mu}$ . Laboratory measurements often provide  $n_{\lambda}$  and  $k_{\lambda}$  for various compounds supposedly present in space.

which is nothing else than the probability per unit length for a photon to interact with a dust grain.

This means that the fraction of intensity lost due to extinction within a length interval dl along the path of travel is:

$$dI_{\lambda} = -\kappa_{\lambda}^{ext} I_{\lambda} dl \tag{1.5}$$

If a source of brightness  $I_0$  exists behind the dust cloud then we can integrate equation 1.5 throughout the cloud and get the intensity I coming out of the cloud:

$$I = I_0 e^{-\tau_\lambda} \tag{1.6}$$

where  $\tau_{\lambda}$  is the optical depth of this cloud:

$$\tau_{\lambda} = \int \kappa_{\lambda}^{ext} \, dl \tag{1.7}$$

Equations 1.6 and 1.7 represent the basics of the radiative transfer process. As we will see in this dissertation, the picture gets complicated with the dust emission and scattering behaving as energy sources for I, as well as with the dust properties being a function of location in the cloud. Nonetheless, it always comes to some form of these equations, as the main goal of any radiative transfer calculation is to calculate how much energy is streaming into a point of space. If we were observers then this information tell us what we measure with our instruments. If we were a dust particle then this energy keeps us warm and regulates our temperature.

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# Chapter 2

# Theory

Radiative transfer equations have been described in detail by many authors. New and innovative ways of rewriting these equations can lead to a better insight and sometimes to a new method of numerical solution. The major progress in radiative transfer solvers has been achieved for the equations in one-dimensional geometries (for a recent review see Peraiah (2002)). The equations in multidimensional geometries are still not fully explored in regard to potential numerical treatments. Especially important is to decide which form of equations to use in the numerical approach: differential, integro-differential, or integral form. As we will argue in the next chapter, there are strong motivations for using the integral form to explore new numerical methods.

This chapter<sup>(1)</sup> deals with the detailed description of the axially symmetric twodimensional equations used in LELUYA. The problems that LELUYA aims to solve can be described with the radiative transfer equation:

$$\frac{dI_{\lambda}}{d\tau_{\lambda}} = S_{\lambda} - I_{\lambda}$$

which is a more general version of equation 1.5. The term  $S_{\lambda}$  represents an energy source due to dust scattering and dust emission processes.  $S_{\lambda}$  is where numerical difficulties are hidden and where details of a particular application enter. This equation will be explored in more detail in the next section. Notice that LELUYA deals with a *steady state* description of radiative transfer: time variation of the intensity does not enter the equation. This assumes that the light travels across the computational domain in a time

<sup>&</sup>lt;sup>(1)</sup>Marked by red color in this chapter are equations written in the form used in LELUYA.

interval much shorter than the timescale of any intensity variation. In other words, time variations in the energy source and/or in the dust density distribution are slow enough that the whole dust cloud reaches a new equilibrium much faster than the timescale of these variations.

One important aspect of our description is the scaling approach, originally described by Ivezić and Elitzur (1997). Thanks to scaling, all but one parameter can be described with dimensionless quantities. Luminosities, units of densities, and linear dimensions are irrelevant, while the only relevant property of the stellar radiation is its spectral shape. By our choice, only the temperature of dust destruction/creation is specified in real units (kelvins). This approach implies general similarities between apparently different objects and can significantly reduce the free-parameter space during modeling. It also helps us to write equations in such a way that during the phase of numerical solver development we can approach them from various aspects without changing them.

### 2.1 Radiative transfer equation

In equation 1.5 we have already described how dust can reduce the intensity  $I_{\lambda}$  along the path dl. Here we add two additional terms that increase the intensity. The first is thermal radiation from the dust itself. Since emission is the inverse process to absorption, the dust emission coefficient  $\kappa_{\lambda}^{em}$  is equal to the absorption coefficient  $\kappa_{\lambda}^{abs}$ . Thus, the contribution to the intensity is  $\kappa_{\lambda}^{abs} B_{\lambda}(T)$ , where  $B_{\lambda}$  is the Planck function and T is the dust temperature. The second additional term is radiation coming from other directions, but accidentally scattered into the direction of dl (described as the unit vector  $\hat{l}$ ). This contribution is  $\kappa_{\lambda}^{sca} J_{\lambda}$ , where  $J_{\lambda}$  is the mean intensity (or angular averaged intensity):

$$J_{\lambda} = \int_{\Omega} I_{\lambda} \ (\theta, \varphi) \frac{d\Omega}{4\pi}$$
(2.1)

for  $d\Omega = \sin\theta d\theta d\varphi$ . In the case of anisotropic scattering we would introduce the angular phase function  $g_i(\Omega, \hat{l})$  for scattering from direction  $\Omega$  to  $\hat{l}$  of the dust type *i*, and the mean intensity would be:

$$J_{\lambda,i} = \int_{\Omega} I_{\lambda} \ (\theta,\varphi) g_i(\Omega,\hat{l}) \frac{d\Omega}{4\pi}$$
(2.2)

Taking into consideration that different dust types i can have different temperatures  $T_i$ , we write the radiative transfer equation as:

$$\frac{dI_{\lambda}}{dl} = -\sum_{i} \kappa_{\lambda,i}^{ext} I_{\lambda} + \sum_{i} \kappa_{\lambda,i}^{abs} B_{\lambda} (T_{i}) + \sum_{i} \kappa_{\lambda,i}^{sca} J_{\lambda}$$
(2.3)

The total extinction coefficient in equation 1.4 helps us to rewrite the transfer equation as:

$$\frac{dI_{\lambda}}{dl} = \kappa_{\lambda}^{ext} \left( \sum_{i} \frac{\kappa_{\lambda,i}^{abs}}{\kappa_{\lambda}^{ext}} B_{\lambda} \left( T_{i} \right) + \sum_{i} \frac{\kappa_{\lambda,i}^{sca}}{\kappa_{\lambda}^{ext}} J_{\lambda} - I_{\lambda} \right)$$
(2.4)

The energy source terms are usually called the *source function*:

$$S_{\lambda} = \sum_{i} \frac{\kappa_{\lambda,i}^{abs}}{\kappa_{\lambda}^{ext}} B_{\lambda} (T_{i}) + \sum_{i} \frac{\kappa_{\lambda,i}^{sca}}{\kappa_{\lambda}^{ext}} J_{\lambda}$$
(2.5)

and, together with the definition of optical depth  $d\tau_{\lambda} = \kappa_{\lambda}^{ext} dl$ , it gives the general form of the radiative transfer equation:

$$\frac{dI_{\lambda}}{d\tau_{\lambda}} = S_{\lambda} - I_{\lambda} \tag{2.6}$$

The source function is what makes the radiative transfer so difficult to solve. The scattering part couples all dust particles to each other through photons bouncing from one particle to another. The dust thermal radiation part is easier to handle if we know the dust temperature. In that case we would need to raytrace the dust cloud just once. Unfortunately, the dust temperature is regulated by the radiation field, thus we do not know the temperature in advance.

### 2.2 Flux and luminosity

Two important quantities that we encounter in astrophysics are the flux and luminosity. The *flux* in direction  $\hat{n}$  is the total energy streaming through a unit surface in a unit time and wavelength:

$$\vec{F}_{\lambda}(\hat{n}) = \hat{n} \int_{\Omega} I_{\lambda}(\theta,\varphi) \hat{n} \cdot d\hat{\Omega} = \int_{\Omega} I_{\lambda}(\theta,\varphi) \cos\theta \, d\Omega \tag{2.7}$$

The same energy integrated over the whole energy spectrum is called the *bolometric flux*:

$$\vec{F}_{bol}(\hat{n}) = \hat{n} \int_{\lambda} \int_{\Omega} I_{\lambda} (\theta, \varphi) \cos \theta \, d\Omega \, d\lambda$$
(2.8)

If we want to see how much energy is coming out of an object, we need to enclose it by a surface and integrate the bolometric flux over this surface. This is called the *luminosity*:

$$L_{\lambda} = \int_{S} \vec{F}_{bol} \cdot d\hat{S} \tag{2.9}$$

The luminosity is a very important quantity for us because it can be used to check the energy conservation. No matter what the shape of the closed integral surface is, the luminosity stays constant as long as the same energy sources are within the surface. A dusty medium enclosed within the surface cannot change this because the extinction processes do not destroy or create energy - they only change its wavelength or direction of travel. In LELUYA, the luminosity over spheres of various radii is calculated to check its conservation. If the temperature iterations converge without achieving luminosity conservation then the numerical grids are too coarse.

## 2.3 Dust temperature and local thermodynamic equilibrium

In order to derive the dust temperature from the local radiation field, we impose the condition of local thermodynamic equilibrium. It states that the dust temperature follows directly form the energy balance between radiative heating and cooling:

$$heating = cooling$$
$$\int \kappa_{\lambda,i}^{abs} J_{\lambda} d\lambda = \int \kappa_{\lambda,i}^{abs} B_{\lambda} (T_i) d\lambda$$
(2.10)

If other forms of heating are also important then they should be included in this equation. In the current version of LELUYA they are neglected, but in the future versions additional heating mechanisms, like viscous heating in dense accretion disks, will be included.

In equation 2.10 we made an assumption that the dust temperature does not fluctuate in time. This means that the time interval between the absorption of energetic photons is larger than the cooling time. "Energetic" means an energy comparable to the heat capacity of a dust grain. When such a photon is absorbed, the temperature jumps abruptly by a K or more. Then it takes some time for the particle to cool down by emitting lowenergy photons. For large particles this does not represent a problem because of their large heat capacity. For nano-size particles, however, equation 2.10 might be too simplistic. The actual size of these small grains depends on the radiation field. If we deal with a "hard" field then even somewhat larger particles will be affected. The field is "weak", when the intervals between capturing photons become too long.

There is a way of treating this stochastic time evolution of dust temperature. The plan is to incorporate it into future versions of LELUYA. So far, equation 2.10 works fine for the currently considered applications. As we already mentioned, the dust temperature  $T_i$  is not known in advance. Thus, we start with an initial guess for  $T_i$ , calculate  $J_{\lambda}$  and then use equation 2.10 to update the temperature. This procedure is iterated until the temperature converges toward one stable value.

### 2.4 Scaling

In their analysis of the radiative transfer equation 2.6, Ivezić and Elitzur (1997) realized that all but one parameter can be described with dimensionless quantities. This scaling property removes the need for real units of luminosity, dust density, linear scales, stellar radiation, and dust extinction coefficients. The temperature of dust destruction/creation is the only dimensional quantity that needs to be specified. Density and distance scales do not enter individually, only indirectly through the overall optical depth. The only relevant property of the stellar radiation is its spectral shape, while the only relevant dust properties are the spectral shapes of the absorption and scattering coefficients. All these aspects of scaling are described in this and forthcoming sections.

Notice that equation 2.10 does not depend on the absolute value of  $\kappa_{\lambda,i}^{abs}$ . We can, therefore, introduce scaling of the absorption coefficients by an arbitrary chosen value. Since we work with a grain mixture, the scaling can be done by one of the components. Let us use  $\kappa_{\lambda,0}^{abs}$ , the absorption coefficient of the first (counting from zero) dust component in the mix at a given wavelength  $\lambda_0$ . In addition, since the extinction coefficients are spatially depended,  $\kappa_{\lambda,0}^{abs}$  is not uniquely specified until we do not specify its exact location.

Thus, before we proceed with our theoretical analysis, we should make one important step of introducing a dimensionless spatial scale. Any vector in 3D space is scaled by some value  $r_1 = |\vec{r_1}|$ . Then we deal only with dimensionless position vectors  $\vec{\rho} = \vec{r}/r_1$ . This specific vector  $\vec{r_1}$  becomes  $\vec{1} = \vec{r_1}/r_1$ , and it is fixed in space. Later on we will see how to choose and calculate this vector.

Unfortunately, considering the possible applications of numerical algorithms, in two and three dimensions we cannot rescale the whole space after each temperature iteration step. This comes from the fact that we do not know *a priori* the dust temperature at  $\vec{l}$ . This is forcing us to anchor the numerical grid to the dust density distribution. That allows us to create or destroy dust at  $\vec{l}$  according to the local dust temperature at that point.

The dust density distribution  $n_i(\vec{\rho})$  and the absorption cross section  $\sigma_{a_{\lambda},i}$  have to be specified beforehand for each dust component *i*, so that the dimensionless extinction coefficients can be derived:

$$q_{\lambda,i}^{abs,sca,ext} = \frac{n_i(\vec{\rho})}{n_0(\vec{1})} \quad \frac{\sigma_{\lambda,i}^{abs,sca,ext}}{\sigma_{\lambda,0}^{abs}}$$
(2.11)

We also need to scale the angle-averaged intensity  $J_{\lambda}$  ( $\vec{\rho}$ ). For this purpose, we introduce the scaling bolometric flux  $F_{norm}$ . Later on we will decide how to define it so that it will be the most convenient for us. The most natural choice would be to use the source bolometric flux  $F_{norm} = L^*/4\pi (r^*)^2$ , where  $r^*$  is the source radius. There is a practical problem, however, when we work with a non-spherical source (e.g. a star or a black hole with a hot accretion disk around it). This choice of  $F_{norm}$  would require the integral over the source surface, which can be very tricky to do numerically. Since we do not want to introduce a large numerical error directly into the definition of equations that we are solving, we will use a different, simplified choice for  $F_{norm}$ . On the other hand, we will need this tricky integral for calculating the source intensity at grid vertices and for luminosity conservation. As all these issues are relevant only for very anisotropic sources, the current version of LELUYA works only with spherical sources where  $F_{norm} = F_{bol}$  anyway.

The scaled intensity becomes:

$$u_{\lambda}\left(\vec{\rho}\right) = \frac{4\pi\rho^2}{F_{norm}} J_{\lambda}\left(\vec{\rho}\right) \tag{2.12}$$

where we use  $\rho = |\vec{\rho}|$ .

Scaling of the Planck function  $B_{\lambda}(T_i(\vec{\rho}))$  is straightforward:

$$b_{\lambda}\left(T_{i}(\vec{\rho})\right) = \frac{\pi B_{\lambda}\left(T_{i}(\vec{\rho})\right)}{\sigma_{SB}T_{i}^{4}(\vec{\rho})} \tag{2.13}$$

where  $\sigma_{SB}$  is the Stefan-Boltzmann constant.  $u_{\lambda}$  and  $b_{\lambda}$  have the units of  $\lambda^{-1}$ , but this does not concern us because it cancels out in all equations where  $u_{\lambda}$  and  $b_{\lambda}$  appear.

## 2.5 Optical depth scale

The general definition of the optical depth along a path  $\mathcal{P}$ , as already described in equation 1.7, is:

$$\tau_{\lambda} (P) = \int_{P} \kappa_{\lambda}^{ext} (r_{1}\vec{\rho}) d(r_{1}\rho) = r_{1} \sum_{i} \int_{P} n_{i}(\vec{\rho}) \sigma_{\lambda,i}^{ext} d\rho$$
(2.14)

From the computational point of view, the preferred choice is a path that gives the largest optical depth through the dusty envelope. This is almost always a radial path and a user will have to specify its azimuthal angle  $\theta_0$ .

The total optical depth  $\tau_{\lambda_0}^T$  at the wavelength  $\lambda_0$  has to be specified, too. This optical depth is a result of extinction between the closest distance to the source  $\rho_{sub}$  (determined by the temperature of dust destruction/creation) and the outer radius of the computational domain  $\rho_{out}$ :

$$\tau_{\lambda_0}^T = r_1 \sum_i \int_{\rho_{sub}}^{\rho_{out}} n_i(\rho, \theta_0) \sigma_{\lambda_0, i}^{ext} d\rho$$
(2.15)

If we take the ratio of the last two equations, the optical depth can be rewritten as:

$$\tau_{\lambda} (P) = \int_{P} \eta_{\lambda}(\vec{\rho}) d\rho \qquad (2.16)$$

where  $\eta_{\lambda}$  is:

$$\eta_{\lambda} \left( \vec{\rho} \right) = \frac{\tau_{\lambda_0}^T \sum_i n_i(\vec{\rho}) \sigma_{\lambda,i}^{ext}}{\sum_j \sigma_{\lambda_0,j}^{ext} \int_{\rho_{sub}}^{\rho_{out}} n_j(\rho, \theta_0) d\rho}$$
(2.17)

 $\eta_{\lambda}$  plays the central role in specifying the problem we are solving. It contains the density and extinction spatial distributions, which is the signature of individual astrophysical environments.
## 2.6 Scaled thermodynamic equilibrium equation

With the scaled values introduced, equation 2.10 becomes:

$$\frac{4\sigma_{SB}T_i^4(\vec{\rho})}{F_{norm}\rho^2} \int q_{\lambda,i}^{abs}(\vec{\rho}) b_\lambda(T_i(\vec{\rho})) d_\lambda = \int q_{\lambda,i}^{abs}(\vec{\rho}) u_\lambda(\vec{\rho}) d\lambda$$
(2.18)

This equation only holds when we have the correct  $T_i(\vec{\rho})$  and  $F_{norm}$ .

We continue with the scaling procedure by introducing:

$$\Psi = \frac{4\sigma_{SB}T_{sub,0}^4}{F_{norm}} \tag{2.19}$$

where  $T_{sub,0}^4$  is the sublimation temperature (at which the dust is destroyed or created) of the  $0^{th}$  dust component. Instead of changing  $F_{norm}$  during the iteration process, we change the dimensionless quantity  $\Psi$ .

Now we can finally rewrite the equilibrium equation 2.18 in the form used in LELUYA:

$$T_{i}^{4}(\vec{\rho}) \int q_{\lambda,i}^{abs}(\vec{\rho}) b_{\lambda}(T_{i}(\vec{\rho})) d\lambda - \frac{T_{sub,0}^{4}}{\rho^{2}\Psi} \int q_{\lambda,i}^{abs}(\vec{\rho}) u_{\lambda}(\vec{\rho}) d\lambda = 0$$
(2.20)

## 2.7 Global iteration loop

Multidimensional radiative transfer brings one additional problem not encountered in one-dimensional geometries. The sublimation cavity is a region of space around the central energy source where the dust cannot exist because it gets too hot. The cavity surface, often called the *sublimation/condensation surface*, is defined by the dust sublimation/condensation temperature. In 1D geometries, we know its shape in advance (a sphere for spherical geometry, or an infinite flat plane for a slab). In multidimensional geometries, however, we do not know it in advance. Instead, it has to be a part of the final solution. If we describe this surface as  $S_{cavity,i}$  for the  $i^{th}$  dust component, and its temperature as  $T(S_{cavity,i})$ , then we have to solve the implicit equation:

$$T(S_{cavity,i}) = T_{sub,i} = constant$$
(2.21)

This is a very serious problem because it says that we cannot even specify the problem we are solving until we know  $S_{cavity,i}$ . There is no radiative transfer code other than LELUYA that can handle this problem. What other codes do is to fix the shape of the cavity and abandoning the premise of having the sublimation/condensation temperature defining its shape. LELUYA, on the other hand, reshapes the surface after each update of the dust temperature.

In order to do that, the scaling point 1 has to be chosen wisely, since the density distribution and the extinction coefficients critically depend on its choice (equation 2.11). The best way is to predict which dust species will be the closest to the source along one radial line, mark this species as the 0<sup>th</sup> component, and then use its sublimation/condensation point on that radial line as  $\vec{1}$ . The default direction is the equatorial plane, but the user can specify any other direction as well.<sup>(2)</sup> An additional consequence of this problem is that the computational grid has to be recalculated after each temperature update. Since the cavity's surface can change during the dust temperature updates, the  $\eta_{\lambda}$  denominator also has to be updated as the surface changes.

The next thing is to figure out how to update  $\Psi$ . We need a point where we keep the dust temperature constant by definition. Since our guess for the closest dust species along the given radial direction might be incorrect, we have to keep open the possibility that other dust species will be closer to the energy source. Thus, before updating  $\Psi$  we have to find the closest point  $\vec{\rho}_{sub}$  to the source along the given radial line. After that, we use this point for updating  $\Psi$ , which will ensure that this point stays exactly at the sublimation/condensation temperature. The updated  $\Psi$  follows from equation 2.20 and becomes:

$$\Psi = \frac{T_{sub,0}^4}{\rho_{sub}^2 T_{sub,j}^4} \quad \frac{\int q_{\lambda,j}^{abs} \left(\vec{\rho}_{sub}\right) u_{\lambda} \left(\vec{\rho}_{sub}\right) d\lambda}{\int q_{\lambda,j}^{abs} \left(\vec{\rho}_{sub}\right) b_{\lambda} \left(T_{sub,j}\right) d\lambda} \tag{2.22}$$

where j is the dust component which exists at  $\vec{\rho}_{sub}$ .

At this stage we can see what the global iteration loop should look like. The only part missing is how to calculate  $u_{\lambda}$  and this will be described in the upcoming sections.

a) find initial  $T_i(\vec{\rho})$ ,  $u_\lambda(\vec{\rho})$ , and  $\Psi$ 

 $<sup>^{(2)}</sup>$ In a spherical geometry, for example, the direction does not matter because  $\vec{1}$  is on a sphere.

- b) find new  $u_{\lambda}$   $(\vec{\rho})$
- c) update  $\eta_{\lambda}$  denominator in equation 2.17
- d) find new  $\Psi$  from equation 2.22
- e) find new dust temperatures  $T_i(\vec{\rho})$  from equation 2.20
- f) update the source size
- g) make corrections of the sublimation surfaces
- h) check convergence
- i) go to b) if the convergence is not achieved

The step (f) is also described in the upcoming sections. The sublimation surface correction is a tricky problem by itself. Resolving it requires numerous "technical" procedures, which go beyond the presentation of this dissertation.

## 2.8 The integral form of radiative transfer

The differential form of the radiative transfer equation 2.6 can be rewritten into an integral form, known as "the formal solution to the radiative transfer problem". The analytical procedure of deriving the formal solution can be found in any advanced book on radiative transfer. In general, the procedure consists of multiplying equation 2.6 by  $e^{-\tau}$  and integrating by parts. If additionally integrated over  $d\Omega$ , the integral form is expressed in terms of the mean intensity  $J_{\lambda}$  instead of the ordinary  $I_{\lambda}$ . It is numerically convenient to distinguish between the intensity contribution  $J^*_{\lambda}$  coming directly from the central source, usually called the *stellar* radiation, and the *diffuse* contribution  $J^{diff}_{\lambda}$  coming from the dust:

$$J_{\lambda} \left( \vec{\rho} \right) = J_{\lambda}^{*} \left( \vec{\rho} \right) + J_{\lambda}^{diff} \left( \vec{\rho} \right)$$

The formal solution, with the source function from equation 2.5 included, is then:

$$J_{\lambda}(\vec{\rho}) = J_{\lambda}^{*}(\vec{\rho}) + \iint \sum_{i} \left[ \frac{\kappa_{\lambda,i}^{abs}(\vec{\rho}')}{\kappa_{\lambda}^{ext}(\vec{\rho}')} B_{\lambda}(T_{i}(\vec{\rho}')) + \frac{\kappa_{\lambda,i}^{sca}(\vec{\rho}')}{\kappa_{\lambda}^{ext}(\vec{\rho}')} J_{\lambda}(\vec{\rho}') \right] e^{-\tau_{\lambda}(\vec{\rho}',\vec{\rho})} d\tau_{\lambda}(\vec{\rho}',\vec{\rho}) \frac{d\Omega_{\vec{\rho}}}{4\pi}$$

$$(2.23)$$

The integral over optical depth is performed on a line defined by the angular direction of  $d\Omega_{\vec{\rho}}$ . A point on that line is  $\vec{\rho'}$  and the optical depth distance to  $\vec{\rho}$  is  $\tau_{\lambda}(\vec{\rho'},\vec{\rho})$ .

The ratio of scattering and total extinction coefficients is called the *albedo*. For the  $i^{th}$  dust component it is given by:

$$\omega_{\lambda,i}(\vec{\rho}) = \frac{\kappa_{\lambda,i}^{sca}(\vec{\rho})}{\kappa_{\lambda,i}^{ext}(\vec{\rho})} = \frac{\sigma_{\lambda,i}^{sca}}{\sigma_{\lambda,i}^{abs} + \sigma_{\lambda,i}^{sca}}$$
(2.24)

and equation (2.23) can be rewritten as:

$$J_{\lambda}(\vec{\rho}) = J_{\lambda}^{*}(\vec{\rho}) + \int \int \sum_{i} \Upsilon_{\lambda,i}(\vec{\rho'}) \left[ (1 - \omega_{\lambda,i}) B_{\lambda}(T_{i}(\vec{\rho'})) + \omega_{\lambda,i} J_{\lambda}(\vec{\rho'}) \right] e^{-\tau_{\lambda}(\vec{\rho'},\vec{\rho})} d\tau_{\lambda}(\vec{\rho'},\vec{\rho}) \frac{d\Omega_{\vec{\rho}}}{4\pi}$$

$$(2.25)$$

where we introduced  $\Upsilon_{\lambda,i}$ :

$$\Upsilon_{\lambda,i}(\vec{\rho}) = \frac{n_i(\vec{\rho})(\sigma_{\lambda,i}^{abs} + \sigma_{\lambda,i}^{sca})\Theta\left(T_{sub,i} - T_i(\vec{\rho})\right)}{\sum_j n_j(\vec{\rho})(\sigma_{\lambda,j}^{abs} + \sigma_{\lambda,j}^{sca})\Theta\left(T_{sub,j} - T_j(\vec{\rho})\right)}$$
(2.26)

 $\Theta(x)$  is the step function (1 for  $x \ge 0$  and 0 for x < 0).

We recognize the source function as:

$$S_{\lambda}(\vec{\rho}) = \sum_{i} \Upsilon_{\lambda,i}(\vec{\rho}) \left[ (1 - \omega_{\lambda,i}) B_{\lambda}(T_{i}(\vec{\rho})) + \omega_{\lambda,i} J_{\lambda}(\vec{\rho}) \right]$$
(2.27)

## 2.9 Stellar contribution to intensity

The stellar part of the formal solution 2.25 at  $\vec{\rho}$  is:

$$J_{\lambda}^{*}\left(\vec{\rho}\right) = \frac{1}{4\pi} \int_{\Omega_{\vec{\rho}}^{*}} I_{\lambda}^{*}(\hat{\zeta}) e^{-\tau_{\lambda}\left(\hat{\zeta}\right)} d\Omega_{\vec{\rho}}^{*}(\hat{\zeta}) \quad (2.28)$$

where  $\Omega_{\vec{\rho}}^*$  is the solid angle of the source surface visible from the point  $\vec{\rho}$ . The unit vector  $\hat{\zeta}$  points to  $\vec{\rho}$  from the stellar surface (see figure 2.1) and  $\tau_{\lambda}(\hat{\zeta})$  is the optical depth between the surface and  $\vec{\rho}$  along the line define



Figure 2.1: From a point  $\vec{\rho}$ , the source (gray ball) has the angular size of  $\Omega^*(\vec{\rho})$ . Any ray between the point  $\vec{\rho}$  and the source surface is defined by a unit vector  $\vec{\zeta}$ .

tween the surface and  $\vec{\rho}$  along the line defined by  $\hat{\zeta}$ . The infinitesimal solid angle  $d\Omega$  is pointing along  $-\hat{\zeta}$  toward a point on the stellar surface of intensity  $I_{\lambda}^*(\hat{\zeta})$ .

If a point  $\vec{\rho}_{\infty}$  is very far away from the source, the source will look like a point. The corresponding "point source" flux along the line of azimuth  $\theta_{\infty}$  is:

$$F^*_{\lambda\infty}(\vec{\rho}_{\infty}) = \int_{\Omega^*_{\vec{\rho}_{\infty}}} I^*_{\lambda}(\hat{\zeta}_{\infty}) \cos\theta' d\Omega^*_{\vec{\rho}_{\infty}}(\theta',\varphi')$$
(2.29)

where  $\theta'$  and  $\varphi'$  are spherical angles around the point  $\vec{\rho}_{\infty}$ , and  $\cos \theta_{\infty} = \hat{z} \cdot \vec{\rho}_{\infty}$ . The source radius  $\rho^* \ll \rho_{\infty}$ , thus:

$$\theta' \approx \frac{\rho^* \sin \gamma}{\rho_\infty} \tag{2.30}$$

where  $\gamma$  is the angle between  $\vec{\rho}_{\infty}$  and the vector toward the point  $\hat{\zeta}_{\infty}(\theta', \varphi')$  on the stellar surface (see figure 2.2). Then  $d\theta' = \cos \gamma d\gamma \rho^* / \rho_{\infty}$ ,  $\cos \theta' \approx 1$ ,  $\sin \theta' \approx \theta'$ , from which  $F^*_{\lambda \infty}$ becomes:

$$F_{\lambda\infty}^*(\vec{\rho}_{\infty}) \approx \left(\frac{\rho^*}{\rho_{\infty}}\right)^2 \int_0^{2\pi} \int_0^1 I_{\lambda}^*(\hat{\zeta}_{\infty}) \cos\gamma \, d\cos\gamma \, d\varphi' \tag{2.31}$$



If the source intensity is uniform all over the surface  $I^*_{\lambda}(\hat{\zeta}_{\infty}) = I^*_{\lambda} = const.$ , then  $F^*_{\lambda\infty}(\vec{\rho}_{\infty}) \approx \pi (\rho^*/\rho_{\infty})^2 I^*_{\lambda}$ , as already described in Ivezić and Elitzur (1997). Therefore, we introduce the *equivalent point source intensity*:

$$I_{\lambda\infty}^*(\theta_{\infty}) = \frac{1}{\pi} \int_0^{2\pi} \int_0^1 I_{\lambda}^*(\hat{\zeta}_{\infty}) \cos\gamma \, d\cos\gamma \, d\varphi'$$
(2.32)

so that  $F^*_{\lambda\infty}(\vec{\rho}_{\infty}) \approx \pi (\rho^*/\rho_{\infty})^2 I^*_{\lambda\infty}(\theta_{\infty}).$ 

Figure 2.2: Watching from  $\vec{\rho}$  far away along a line of azimuth  $\theta_0$ , the source looks like a point and the rays are almost parallel. The source surface angle between the ray  $\hat{\zeta}$  and the vector  $\vec{\rho}$  is  $\gamma$  (see text).



$$I_{\lambda\infty}^* = 2 \int_0^1 I_{\lambda}^* (\theta, \hat{z}) \cos\theta \, d\cos\theta \tag{2.33}$$

This "synthetic" intensity is used for scaling the "real" source intensity  $I_{\lambda}^{*}(\hat{\zeta})$  in equation 2.28:

$$i_{\lambda}^{*}(\hat{\zeta}) = \frac{I_{\lambda}^{*}(\bar{\zeta})}{I_{\lambda\infty}^{*}}$$
(2.34)

and  $I^*_{\lambda\infty}$  can be taken out from the integral in equation 2.28, together with the optical depth  $\tau_{\lambda}(\vec{\rho})$ :

$$J_{\lambda}^{*}\left(\vec{\rho}\right) = \frac{I_{\lambda\infty}^{*}}{4\pi} e^{-\tau_{\lambda}\left(\vec{\rho}\right)} \int_{\Omega_{\vec{\rho}}^{*}} i_{\lambda}^{*}(\hat{\zeta}) e^{-(\tau_{\lambda}\left(\hat{\zeta}\right) - \tau_{\lambda}\left(\vec{\rho}\right))} d\Omega_{\vec{\rho}}^{*}(\hat{\zeta})$$
(2.35)

Here we can see the purpose of this rewritten equation for  $J_{\lambda}^{*}(\vec{\rho})$ . The part of equation out of the integral does not depend explicitly on the source size, while the integral represents a correction to this point source approximation. In other words, if we introduce the mean equivalent point source intensity:

$$J_{\lambda\infty}^*(\vec{\rho}) = \frac{1}{4} \left(\frac{\rho^*}{\rho}\right)^2 I_{\lambda\infty}^* e^{-\tau_\lambda (\vec{\rho})}$$
(2.36)

then we can rewrite equation (2.35):

$$J_{\lambda}^{*}\left(\vec{\rho}\right) = J_{\lambda\infty}^{*}\left(\vec{\rho}\right)\xi_{\lambda}^{*}\left(\vec{\rho},\rho^{*}\right) \tag{2.37}$$

where we use:

$$\xi_{\lambda}^{*}(\vec{\rho},\rho^{*}) = \frac{1}{\pi(\rho^{*}/\rho)^{2}} \int_{\Omega_{\vec{\rho}}^{*}} i_{\lambda}^{*}(\hat{\zeta}) e^{-(\tau_{\lambda}(\hat{\zeta})-\tau_{\lambda}(\vec{\rho}))} d\Omega_{\vec{\rho}}^{*}(\hat{\zeta})$$
(2.38)

(keep in mind that  $\Omega_{\vec{\rho}}^*$  also depends on  $\rho^*/\rho$ ). Notice that  $I_{\lambda\infty}^*$  needs to be calculated only once, before the iterations start, and it is used just to scale the other intensities.

What about non-spherical sources? The procedure is the same, except that we have to be careful with the angular integration. In case of  $I_{\lambda\infty}^*$  we consider only intensities  $I_{\lambda}^*(\theta, \hat{z})$ which originate from the source surface. But in equation 2.38 the source intensity can be also a diffuse radiation behind the sphere of radius  $\rho^*$  if the angular ray of integration does not intersect the non-spherical source. Thus, in general, equation 2.38 is potentially difficult for numerical integration in cases of extremely complex energy sources.

## 2.10 Scaled radiative transfer

The scaled intensities in equation 2.12 and 2.13 can be used for deriving the scaled source function  $s_{\lambda}(\vec{\rho})$  from equation 2.27:

$$s_{\lambda}\left(\vec{\rho}\right) = \sum_{i} \Upsilon_{\lambda,i}(\vec{\rho}) \left[ (1 - \omega_{\lambda,i}) \Psi \rho^2 \left(\frac{T_i(\vec{\rho})}{T_{sub,0}}\right)^4 b_{\lambda} \left(T_i\left(\vec{\rho}\right)\right) + \omega_{\lambda,i} u_{\lambda}\left(\vec{\rho}\right) \right]$$
(2.39)

The scaled radiative transfer solution is then:

$$u_{\lambda}(\vec{\rho}) = \frac{4\pi\rho^2}{F_{norm}} J^*_{\lambda\infty}(\vec{\rho}) \,\xi^*_{\lambda}(\vec{\rho},\rho^*) + \iint \left(\frac{\rho}{\rho'}\right)^2 s_{\lambda}(\vec{\rho'}) \,e^{-\tau_{\lambda} \,(\vec{\rho'},\vec{\rho})} d\tau_{\lambda}(\vec{\rho'},\vec{\rho}) \,\frac{d\Omega_{\vec{\rho}}}{4\pi} \tag{2.40}$$

Remember that we still have not decided how to define  $F_{norm}$ . The stellar part in the equation above is:

$$\frac{4\pi\rho^2}{F_{norm}}J^*_{\lambda\infty}(\vec{\rho})\,\xi^*_{\lambda}\!(\vec{\rho},\rho^*) = (\rho^*)^2\,\frac{\pi I^*_{\lambda\infty}}{F_{norm}}\,e^{-\tau_\lambda\,(\vec{\rho})}\xi^*_{\lambda}\!(\vec{\rho},\rho^*) \tag{2.41}$$

and it comes naturally to define  $F_{norm}$  as:

$$F_{norm} = \pi (\rho^*)^2 \int I^*_{\lambda \ \infty} d_{\lambda}$$
(2.42)

Finally, we can write the final form of the formal solution from equation 2.40:

$$u_{\lambda}(\vec{\rho}) = f^*_{\lambda\infty} e^{-\tau_{\lambda}(\vec{\rho})} \xi^*_{\lambda}(\vec{\rho}, \rho^*) + \iint \left(\frac{\rho}{\rho'}\right)^2 s_{\lambda}(\vec{\rho'}) e^{-\tau_{\lambda}(\vec{\rho'}, \vec{\rho})} d\tau_{\lambda}(\vec{\rho'}, \vec{\rho}) \frac{d\Omega_{\vec{\rho}}}{4\pi}$$
(2.43)

where  $f^*_{\lambda\infty} = I^*_{\lambda\infty} / \int I^*_{\lambda\infty} d\lambda$  is the spectral shape of  $I^*_{\lambda\infty}$ .

## 2.11 The source luminosity and angular size

In general, "source" is the smallest sphere that confines all central energy sources. The source luminosity is:

$$L^* = \int d\theta \, d\varphi |\vec{r}^*(\theta,\varphi)|^2 \sin\theta \int d\lambda \int d\Omega_{\vec{r}^*}(\hat{\zeta}) I^*{}_{\lambda} \, (\vec{r}^*,\hat{\zeta}) \hat{r^*} \cdot \hat{\zeta}$$
(2.44)

where  $\bar{r}^*(\theta, \varphi)$  (unit vector  $\hat{r}^*$ ) is a radial vector toward a point on the surface of spherical coordinates  $(\theta, \varphi)$ .

This equation can be rewritten as:

$$L^* = 2\left(\frac{r^*}{\rho^*}\right)^2 F_{norm} \int \sin\theta d\theta \int d\lambda f^*_{\lambda\infty} \int d\Omega_{\vec{r^*}}(\hat{\zeta}) i^*_{\lambda}(\vec{r^*},\hat{\zeta}) \hat{r^*} \cdot \hat{\zeta}$$
(2.45)

and by using equation 2.19 we can derive connection between the luminosity and the angular source size:

$$(\rho^*)^2 = \frac{16\pi\sigma_{SB}(r^*)^2 T_{sub,0}^4}{\Psi L^*} \mathcal{L}$$
(2.46)

where  $\mathcal{L}$  has to be calculated only once, before we start with the radiative transfer iterations:

$$\mathcal{L} = \frac{1}{2\pi} \int_{-1}^{1} d\cos\theta \int d\lambda f^*_{\lambda\infty} \int d\Omega_{\vec{r}^*}(\hat{\zeta}) i^*_{\lambda}(\vec{r}^*,\hat{\zeta}) \, \hat{r}^* \cdot \hat{\zeta}$$
(2.47)

As we can see, the user will have to specify the source luminosity  $L^*$  and its size  $r^*$ . When the final solution is reached, the spatial dust density scale in real units can be obtained from  $r_1 = r^* / \rho^*$ .

## 2.12 Luminosity conservation



Figure 2.3: Luminosity is calculated over a sphere of radius  $\rho$  from the radial fluxes  $\vec{F}_{\lambda}(\vec{\rho})$ .

Luminosity conservation is an important component of radiative transfer. In addition to the overall numerical precision, it gives us information about local deviations from the energy conservation. Such a deviation can be a result of a coarse spatial grid, if the energy is missing locally, or a coarse angular grid, if the energy is increased. A simple way of isolating portions of the computational domain is by spheres of various radii centered at the star (central energy source). The luminosity from these spheres should stay equal to the source luminosity 2.45.

Following definitions of flux in 2.7 and lu-

minosity in 2.9, we derive the luminosity of a sphere of radius  $\rho$ :

$$L(\rho) = \iint \vec{F}_{\lambda}(\vec{\rho}) \cdot d\vec{S} \, d\lambda = 4\pi r_1^2 \rho^2 \int_{\lambda} \int_{0}^{\pi/2} F_{\lambda}(\vec{\rho}) \sin\theta \, d\theta \, d\lambda \tag{2.48}$$

where  $d\vec{S}$  is an area element on the sphere.  $\vec{F}_{\lambda}(\vec{\rho})$  is the radial flux on the sphere's surface in the radial direction  $\hat{\rho}$ :

$$\vec{F}_{\lambda}\left(\vec{\rho}\right) = \hat{\rho} \int I_{\lambda}\left(\vec{\rho},\hat{\Omega}\right) \,\hat{\rho} \cdot d\vec{\Omega} \tag{2.49}$$

where the intensity  $I_{\lambda}(\vec{\rho}, \hat{\Omega})$  is streaming into the point  $\vec{\rho}$  from direction  $\hat{\Omega}$ .

Notice that the mean intensity is based on the integral over  $d\Omega$  while the value of flux is based on the integral over  $\hat{\rho} \cdot d\vec{\Omega}$ . Hence, in order to derive the scaled flux  $F_{\lambda}(\vec{\rho})$  we can follow the same procedure as for the mean intensity, except for  $d\Omega$  replaced with  $\hat{\rho} \cdot d\vec{\Omega}$ . The luminosity equation 2.48 is then transformed into:

$$\frac{L(\rho)}{4\pi r_1^2 F_{norm}} = constant = \int_0^1 d\cos\theta \int_{\lambda} d\lambda \bigg[ f^*_{\lambda\infty} e^{-\tau_{\lambda} (\vec{\rho})} \xi^*_{F,\lambda} (\vec{\rho}, \rho^*, \hat{\rho}) + \int_0^1 d\cos\theta \int_{\lambda} d\lambda \bigg[ f^*_{\lambda\infty} e^{-\tau_{\lambda} (\vec{\rho})} \xi^*_{F,\lambda} (\vec{\rho}, \rho^*, \hat{\rho}) + \int_0^1 d\cos\theta \int_{\lambda} d\lambda \bigg[ f^*_{\lambda\infty} e^{-\tau_{\lambda} (\vec{\rho})} \xi^*_{F,\lambda} (\vec{\rho}, \rho^*, \hat{\rho}) + \int_0^1 d\cos\theta \int_{\lambda} d\lambda \bigg[ f^*_{\lambda\infty} e^{-\tau_{\lambda} (\vec{\rho})} \xi^*_{F,\lambda} (\vec{\rho}, \rho^*, \hat{\rho}) \bigg] d\lambda$$

$$+ \int \int \left(\frac{\rho}{\rho'}\right)^2 s_{\lambda}(\vec{\rho'}) e^{-\tau_{\lambda} (\vec{\rho'},\vec{\rho})} d\tau_{\lambda}(\vec{\rho'},\vec{\rho}) \frac{\hat{\rho} \cdot d\vec{\Omega}_{\vec{\rho}}}{4\pi} \right] \quad (2.50)$$

where  $\xi_{F,\lambda}^*$  is (notice how it differs from  $\xi_{\lambda}^*$  in equation 2.38):

$$\xi_{F,\lambda}^*(\vec{\rho},\rho^*,\hat{\rho}) = \frac{1}{\pi(\rho^*/\rho)^2} \int_{\Omega_{\vec{\rho}}^*} i_{\lambda}^*(\hat{\zeta}) e^{-(\tau_{\lambda}(\hat{\zeta}) - \tau_{\lambda}(\vec{\rho}))} \hat{\rho} \cdot d\vec{\Omega}_{\vec{\rho}}^*(\hat{\zeta})$$
(2.51)

When there is no dust, that is no diffuse radiation, the luminosity is equal to  $4\pi r_1^2 F_{norm}$ .

### 2.13 Radiation pressure force

In one-dimensional geometries, the radiation pressure force has only one pre-defined direction. Multidimensional geometries make this direction unknown. The force in direction  $\hat{n}$  is derived from the flux  $\vec{F}_{\lambda}(\vec{\rho}, \hat{n})$ :

$$\vec{\mathcal{F}}(\vec{\rho},\hat{n}) = \frac{1}{c} \int \kappa_{\lambda}^{ext}(\vec{\rho}) \ \vec{F}_{\lambda}(\vec{\rho},\hat{n}) \ d\lambda$$
(2.52)

where c is the speed of light. We can combine the scaled flux from equation 2.50 and  $\eta_{\lambda}$  from equation 2.17 to obtain the scaled radiation pressure force:

$$\frac{cr_{1}\mathcal{F}(\vec{\rho},\hat{n})}{F_{norm}} = \int_{\lambda} \eta_{\lambda}(\vec{\rho}) \left[ \frac{F_{\lambda}(\vec{\rho},\hat{n})}{F_{norm}} \right] d\lambda = \int_{\lambda} d\lambda \frac{\eta_{\lambda}(\vec{\rho})}{\rho^{2}} \left[ f_{\lambda\infty}^{*} e^{-\tau_{\lambda}} (\vec{\rho}) \xi_{F,\lambda}^{*}(\vec{\rho},\rho^{*},\hat{n}) + \int_{\lambda} \int_{\lambda} \left( \frac{\rho}{\rho'} \right)^{2} s_{\lambda}(\vec{\rho'}) e^{-\tau_{\lambda}} (\vec{\rho'},\vec{\rho}) d\tau_{\lambda}(\vec{\rho'},\vec{\rho}) \frac{\hat{n} \cdot d\vec{\Omega}_{\vec{\rho}}}{4\pi} \right]$$
(2.53)

For example, it is useful to calculate the radial and tangential component of the pressure force to see how much is the dust pushed to move around the central source.

## 2.14 Point source approximation

We can safely approximate the central source with a point if the dust cavity surface is at least a few source radii away from the central energy source and without density features on the scale smaller than the source size. The equations are somewhat simplified and take the form presented in Ivezić and Elitzur (1997). Some source-related quantities disappear within this approximation:  $I^*_{\lambda\infty} = I^*_{\lambda}$ ,  $i^*_{\lambda}(\hat{\zeta}) = 1$ , which gives  $\xi^*_{\lambda} = 1$ ,  $\xi^*_{F,\lambda} = 1$  and  $\mathcal{L} = 1$ . The iteration step with calculation of the source size is not required any more. We need only to calculate  $\Psi$ .  $F_{norm}$  becomes  $F_{norm} = L^*/4\pi r_1^2$ . The formal solution of the radiative transfer problem becomes:

$$u_{\lambda}(\vec{\rho}) = f^*_{\lambda\infty} e^{-\tau_{\lambda}(\vec{\rho})} + \iint \left(\frac{\rho}{\rho}\right)^2 s_{\lambda}(\vec{\rho}) e^{-\tau_{\lambda}(\vec{\rho},\vec{\rho})} d\tau_{\lambda}(\vec{\rho},\vec{\rho}) \frac{d\Omega_{\vec{\rho}}}{4\pi}$$
(2.54)

When the central source is a black body of temperature  $T_{eff}$ , the source radius becomes:

$$(\rho^*)^2 = \frac{4}{\pi} \left(\frac{T_{sub,0}}{T_{eff}}\right)^4 \tag{2.55}$$

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# Chapter 3

# Numerical algorithms and software development

## **3.1** General introduction to discretization

The first step in any numerical approach to the radiative transfer is *discretization of the equations* to transform them from a continuum description into a discrete description, replacing derivatives by differences. If the discretization is performed poorly, the obtained difference equations will contain large intrinsical errors. No matter what we do with such equations later on, the final outcome is unlikely to be correct. Hence, due to its complexity and importance, the branch of numerical mathematics dealing with the discretization problems has become a large "industry", meaning both a large field of study and an important component of the modern industrial production line. In general, a discretization covers the computational domain with discrete points that can be connected into a network of discrete cells. The *point discretization* represents the equations at the points, while the *cell discretization* is using cells for that.

When dealing with the points, the solution variables are interpolated from one point to another by polynomials. This is known as the *finite difference* method. There are many ways how to choose the polynomials and points. Since the source function (equation 2.5) couples all points with each other (with dust scattering creating even bigger problems, as described below), a widely popular approach is to couple only adjacent grid points. The influence of points separated by large distances is incorporated through iterative propagation of the solution from one side of the computational domain to another and back, until the solution converges. This is the basic idea behind the *short characteristic* method. If various problems with the convergence and errors are to be avoided, this method has to be applied carefully, with special attention given to the boundary conditions, the difference equations, and the grid structure. All this implies limited capability of the algorithm, with too simplistic computational grids for the applications of our interest. These grids are structured, with pre-defined shape of the cells. The preferred structures are *logically* rectangular (e.g. Dullemond and Turolla 2000, van Noort, Hubeny and Lanz 2002), where "logically" indicates that cylindrical or spherical or polar grids are not different from a rectangular grid from the programming standpoint - only the discretization equations are changed. When faced with steep gradients or strong anisotropies, these grids are an a priori limit to the applicability of the method. In the best case, they are adaptive, where the cell size varies locally, but adaptive grids produce large errors if not refined carefully, forcing the introduction of radiative transfer approximations (Bruls, Vollmöller and Schüssler 1999). Recently, a more clever way of grid refinement was proposed by Steinacker et al. (2003), achieving fairly good results with this approach. Nonetheless, it is still limited in its applicability as it creates an unreasonably large number of grid points in complex geometries and works only for moderately anisotropic radiation fields. Under certain conditions, the method cannot conserve luminosity even though all variables converge.

Among the cell discretization methods we have a choice between the *finite element* method, where the solution variables are represented by a set of trial functions over the cell, and the *finite volume* method, where the energy is exchanged through the cell sides with the solution variables constant within the cell. The Monte Carlo methods are based on the finite volume method, while the finite element methods are not so often used and are not a good choice for highly anisotropic problems with very steep gradients (Richling et al. 2001).<sup>(1)</sup>

The next a priori difficulty of radiative transfer is the question: what form of the

<sup>&</sup>lt;sup>(1)</sup>There is one general numerical approach that has not been explored enough in radiative transfer problems, even though it has a lot of potential: *multi-grid methods*. These methods use grids of various coarseness to reduce the numerical error through interpolating the solution from one grid coarseness level to another (Steiner 1991; Bendicho, Bueno and Auer 1997).

equations should we use for the discretization? We have already mentioned in chapter 2 that we are going to use the integral form called the formal solution (equation 2.23), but a valid question would be why not use the integro-differential form in equation 2.6, or even the flux-version of this equation (see equation 2.7).<sup>(2)</sup> Indeed, these forms are the preferred choice by other authors because there are many numerical methods already developed that can be modified for this purpose. A big drawback of any differential equation, however, is that a derivative of any smooth function oscillates much faster than the function itself. The flux is even worse because it also has a strong directional variation. These are not so serious problems if we deal with slightly or even moderately anisotropic radiation fields, but the anisotropies can be huge for the set of problems that we are targeting.

Dust scattering is generally a numerical nuisance. It makes the radiative transfer equations implicit, with the intensity appearing in the source function through the mean intensity  $J_{\lambda}$  (equation 2.2).  $J_{\lambda}$  is complicated because it couples the solution at one point in the computational domain with the solution at all other points within the whole volume of the domain. The well known and extensively studied method of solving the implicit radiative transfer equations is the *lambda iteration scheme*:  $J_{\lambda} = \Lambda[S_{\lambda}]$ , where  $\Lambda$  operator (think of it as a big matrix) indicates whatever numerical procedure we use in order to obtain  $J_{\lambda}$  from the source function  $S_{\lambda}$ .<sup>(3)</sup> As always with iteration schemes, there is a concern of slow convergence. This led to the *accelerated lambda iteration*, an approximation to the  $\Lambda$  operator which can be more easily inverted and provides faster convergence.

We abandoned the concept of solving the scattering part of radiative transfer iteratively. This is possible if  $\Lambda$  is split into two parts called  $\mathcal{A}$  and  $1 \cdot \mathcal{B}$  (1 is the unit matrix,  $\mathcal{B}$  is a vector). The former is a  $N \times N$  correlation matrix which couples N grid points through dust scattering. The latter depends on the dust temperature and the central

<sup>&</sup>lt;sup>(2)</sup>Radiative transfer equations involving derivatives of  $J_{\lambda}$  and  $F_{\lambda}$  are called the  $\theta^{th}$  and  $1^{st}$  moment equations. The  $3^{rd}$  moment involves the radiation (electromagnetic) pressure tensor. These equations can be derived from equation 2.6 by integration over  $\cos^n \theta d \cos \theta$ , where *n* indicates the equation's moment. The problem, however, with these moment equations is that there is always one unknown variable more than the number of available equations. This is a so-called *closure problem* and it comes down to not knowing  $I_{\lambda}$ .

<sup>&</sup>lt;sup>(3)</sup>In general, the lambda iteration is used with or without the scattering if we consider the implicit  $J_{\lambda}$  through equation 2.10.

energy source. Then we can move  $\mathcal{A}[J_{\lambda}]$  to the left-hand side of the radiative transfer equation and end up with:

$$(1 - \mathcal{A})[J_{\lambda}] = \mathcal{B} \tag{3.1}$$

The matrix  $1 - \mathcal{A}$  is calculated together with the vector  $\mathcal{B}$  and then simply inverted to directly obtain  $J_{\lambda}$  - no iterations needed. Several authors used this method for stellar atmospheres (Gebbie 1967, Kurucz 1969, see also Peraiah 2002 p.82). Kurucz (1969) in his abstract emphasizes: "This method leads to a rapid solution of the integral equation for the source function and to an efficient calculation of the mean intensity and flux.", while Peraiah (2002, p.83) says: "Unlike the iteration method, this gives a direct solution of the integral equation and is therefore free of the difficulties faced in the iteration procedure."

This approach is also used in DUSTY by Ivezić, Nenkova and Elitzur (1999) and it works very efficiently in 1D, with the additional advantage of better and simpler error control. The drawback, however, is that we are forced to use the *long characteristics* method where a grid point is coupled with all other grid points - numerically very expensive task to calculate. Of course, it is not really necessary to couple exactly each single grid point to each other, but the computation is substantial even with a list of speed-up algorithms which avoid many couplings. The main computational effort is to calculate the matrix elements of  $\mathcal{A}$  and, therefore, smaller N is computationally preferable. A smaller number of grid points is also advantageous from the computer memory point of view.

It has to be emphasized here that the final decision about what numerical approach to use is always based on:

- the geometrical complexity of considered problem
- our choice of the required final numerical precision/resolution
- available computer power
- algorithm's complexity from the programming standpoint
- available manpower to perform the programming and computations
- the total time available for such a project

Our initial motivation was to develop a general 2D code for radiative transfer without a priori limits on its applicability, that would permit high numerical precision and spatial resolution. It was clear from the beginning that such a goal is unreachable if we put a strong limit on the computer power. Hence, we abandoned the idea of using a single processor machine and started exploring the parallelization methods to utilize multiprocessor machines.

## **3.2** Basics of the LELUYA's algorithms

We wish to study dust distributions for which the spatial scale and the optical depth scale may change by many orders of magnitude within the computational domain. For example, the typical optical depths in a circumstellar disk around a young PMS star span over six orders at visual wavelengths, while the spatial resolution changes may be even more than that between the outer and inner parts of the disk. Inability to solve the radiative transfer equation for such dust density configurations forced astronomers to use simplified models, which can often lead to very misleading conclusions.



Figure 3.1: Diagram of the LELUYA's main iteration loop.

We decided to explore ways to build an unstructured grid that could map any kind of 2D dust distribution up to a given resolution. This is a difficult task because the grid has to map not only dust density gradients, but also the optical depth. Our goal of having a robust algorithm that can handle anything axially symmetric of arbitrary large optical depth required a completely new approach to the multidimensional radiative

transfer. The existing industry of grid generation methods is based on various types of differential equations where the grid has to map a given function (a scalar or vector). In contrast, the optical depth is a 3D integral function unique to any point in space. The



Figure 3.2: A sequence of steps in the grid generation. A triangle is refined until a certain resolution criterium is reached. If there is a sharp transition from one dust type (shaded area) to another, the grid will trace the edge.

problem remains even if we write the radiative transfer equation in its differential form (moments of the intensity) because the optical depth still enters the equation.

Overall, we had to invent several new algorithms since nothing similar to our unstructured grid has ever been tried before in the radiative transfer techniques. The new algorithms include a **spatial grid generator** (which is the key element for the success of our method), an **angular grid generator**, a **radiative transfer method**, a **parallelization technique**, and even a **way of calculating the final output results**.

The overall problem to solve actually consist of four parts (figure 3.1). The first step is to calculate the correlation matrix  $\mathcal{A}_{\lambda}$  and the thermal emission  $\mathcal{B}_{\lambda}$  (which also includes the attenuated stellar radiation) at each grid point j and wavelength  $\lambda$ . This is the radiative transfer part, where the goal is to find the mean intensity  $J_{\lambda,j}$ . The next step is to deduce the new dust temperatures  $T(\vec{r}_j)$  based on  $J_{\lambda,j}$  and the absorption coefficient  $\kappa_{\lambda,j}^{abs}$ . It is followed by a test of luminosity conservation throughout the computational domain in order to check if the correct solution is reached within a predefined numerical precision. Finally, the fourth step is to check if the dust has to be created or destroyed in or around the sublimation cavity in 2D space. Then a new grid is created and the whole process is repeated until the temperature converges. The required numerical precision is often achieved already after three iteration steps. To make sure that the optimal grid is achieved, calculations with various grid coarseness should be performed and their results compared.



Figure 3.3: Discretization of an optical depth integral (white line). Red triangles indicate locations of grid points (corresponding to triangle vertices) used for the integral interpolation.

LELUYA expects the user to specify the central energy source, that is the shape of its spectrum. It also needs the chemical and physical properties for each dust component, the dust sublimation temperatures, the axially symmetric dust density distribution and the total optical depth at one wavelength along one radial ray. The output result consists of the spectral energy distribution for arbitrary inclination angles, together with 2D images at arbitrary wavelengths, the dust temperature distribution and the bolometric flux at various radii and inclination angles (also used for calculating the luminosity).



Figure 3.4: Same as figure 3.3.

#### 3.2.1 Spatial grid generation

The grid generator has to create an optimal number of points considering gradients of two types of very different physical quantities: the dust density and the optical depth. It starts with a regular hexagonal grid and refines it recursively until a certain resolution criterium is reached. For example, the optical depth is calculated along the sides of triangles and compared with the optical depth toward the edge of dust distribution. The triangle is split into four smaller triangles if the optical depth along its sides is too big. After this recursive process is finished, sharp edges of the dust distribution are identified. In the end, all vertices are interconnected to form a triangular grid (Figure-3.2). One example of a grid used in real life for modelling an AGB star you can see in the next chapter (Figure 4.2).

The relationship between the spatial and optical depth resolution is a complicated nonlinear function of the spatial and optical depth distance toward the dust edge. This function is crucial for achieving desired numerical precision with a relatively small number



Figure 3.5: An angular grid on a unit half-sphere. The area of these spherical triangles is used as a weight factor for the integrals along the lines through the center of triangles.

of points (several thousands).

Spatial grid enables discretisation of the optical depth integral in equation 2.43:

$$\int \left(\frac{\rho}{\rho_{\prime}}\right)^{2} s_{\lambda}(\vec{\rho_{\prime}}) e^{-\tau_{\lambda}(\vec{\rho_{\prime}},\vec{\rho})} d\tau_{\lambda}(\vec{\rho_{\prime}},\vec{\rho}) \to \sum_{j} \left(\frac{\rho}{\rho_{j}}\right)^{2} e^{-\tau_{\lambda}(\vec{\rho_{j}},\vec{\rho})} \Delta \tau_{\lambda}(\vec{\rho_{j}},\vec{\rho}) \times s_{\lambda}(\vec{\rho_{j}})$$
(3.2)

along any line in 3D space starting from the grid point at  $\vec{\rho}$  and ending at the edge of computational domain.

Thanks to axial symmetry, the point  $\vec{\rho_j}$  in 3D space can be described with just two spatial coordinates. This point does not correspond to any grid point because it is highly unlikely that an arbitrary line will go exactly through a grid point. Hence, its properties are interpolated from the vertices of the grid triangle which contains  $\vec{\rho_j}$ . Figure 3.3 and figure 3.4 visualize this situation for one line. Optical depth steps  $\Delta \tau_{\lambda}(\vec{\rho_j}, \vec{\rho})$  are determined from the size of the triangle which contains  $\vec{\rho_j}$ .

#### 3.2.2 Angular grid generation

In order to calculate how much energy is streaming from all directions into one dusty point in space, we have to integrate throughout the whole computational domain volume. This can be a cumbersome job if the number of rays is not optimized. The angular distribution of these rays has to predict the directions where most of the energy is coming from and resolve these sources. A uniform distribution of rays is a bad choice because the angular size of energy sources is usually very small and can not be resolved with a uniform grid without having many thousands of unnecessary rays.

The search starts with an icosahedron and continues recursively dividing the spherical triangles on a unit half-sphere (the full sphere is not needed because of the axial symmetry). The area of these triangles is used as a weight factor  $\Delta W$  in the sum that represents the angular integral over  $4\pi$  steradian:

$$\int_{4\pi} f(\Omega) d\Omega \to \sum_{i} f(\Omega_i) \Delta \Omega_i$$
(3.3)

The integral rays are going through the center of the triangles. A clever method has to be invented for deciding which spherical triangles to split to achieve the optimal angular grid. The numerically most precise algorithm so far takes a 3D distribution of grid points in space and counts how many of them are visible through a spherical triangle. The goal is to have an approximately equal number of grid points visible through each spherical triangle. This approach works because of the way the grid points are distributed in the spatial grid. Their angular distribution around any point in space shows directions of the density and optical depth gradients, which also indicates where to expect the light intensity concentration. An example of an angular grid is shown on Figure-3.5.

Spatial discretization in equation 3.2 combined with angular discretization in equation 3.3 leads to the complete discretization of the optical depth integral (equation 2.43):

$$\iint \left(\frac{\rho}{\rho'}\right)^2 s_{\lambda}(\vec{\rho'}) e^{-\tau_{\lambda}(\vec{\rho'},\vec{\rho})} d\tau_{\lambda}(\vec{\rho'},\vec{\rho}) \frac{d\Omega_{\vec{\rho}}}{4\pi} \to \sum_{i} \sum_{j} \left(\frac{\rho}{\rho_{ij}}\right)^2 e^{-\tau_{\lambda}(\vec{\rho_{ij}},\vec{\rho})} \Delta \tau_{\lambda}(\vec{\rho_{ij}},\vec{\rho}) \frac{\Delta\Omega_{i}}{4\pi} \times s_{\lambda}(\vec{\rho_{ij}})$$
(3.4)

#### **3.2.3** Parallelization efforts

Parallelization in purely radiative transfer codes is not very common. The main reason is a wide use of 1D codes that perform well on single processor machines, while the multidimensional codes are still not so developed. Parallelization is usually performed on the wavelength grid, since each of about 100 wavelengths requires the radiative transfer treatment on its own. We tried that approach, but the processor loads were highly unbalanced and created a lot of idle time.



Figure 3.6: The performance of LELUYA for a small size model (a subiteration over  $\sim 1000$  vertices in an iteration over  $\sim 7000$  in total). Calculations performed on the HP Superdome at UKY with the version of LELUYA as of mid July, 2002.

Thus we use a new approach, where processors work on calculating different rows of the correlation matrix. The scalability of this method is still under investigation, and in figure 3.6 you can see how it currently scales with the number of processors. In addition, calculation of the luminosity conservation is parallelized separately. We also expect to parallelize the parts of the code where the output images and spectrum are calculated.

## **3.3** Computational demands

The overall performance of LELUYA mainly depends on the total number of spatial grid vertices. There is no a simple rule-of-thumb a priori estimate on this number for a given dust geometry and desired numerical precision. A small size problem has about 2000 vertices at the wavelengths with the highest optical depths. A medium size problem requires about 6000 such vertices, while a large (most difficult) problem can go up to 10000.

LELUYA has been under development for the last five years. Even though a large part of the code is still missing, such as the graphic user interface, the priority was to make it operational as soon as possible. The first scientific results are described in the next chapter. There are several additional challenging physical models scheduled for run. The prospective results are of great interest for this field of study. We already have requests for adding additional physics in LELUYA to attack even more challenging problems.

There has been a number of optimization efforts done since LELUYA produced the first useful scientific results. LELUYA's algorithms are new, not fully explored so far, and there is a space for improvements. The most of the improvements, however, depend on the type of a problem that LELUYA is working on. Thus, the real life applications of the code will also yield its best performance.

In a typical modelling of an astrophysical object, we have to run many models before we are able to fit the data. The usual strategy with the 1D codes is to scan the parameter space and often produce many thousands of models. With the multidimensional codes, however, this is not possible because of the large computational demands. The approach has to be different. Thus, it is advisable to study objects with enough data available to a priori reduce the number of modeling free parameters to the minimum. A new model is calculated only when a complete analysis of the previously calculated models is completed. This helps us to anticipate certain results from the next model, hence avoiding unnecessary computations. In the case of CIT3, for example, this approach resulted in 12 runs. The final runs are usually with increased resolution and precision because they require more CPU time.

Another research approach is to study models that are interesting from the theoretical point of view. Each single run of these models is a case study in itself. We plan to use this approach on the flared disk models. These models are usually with a high resolution and medium size grids (around 6,000 vertices), thus computationally the most challenging task for LELUYA so far.

Before engaging in a computational run, we have to be sure that the code will not overflow the available computer memory. The memory peak-requirement follows this equation:

$$Memory[Bytes] = N_{v,max}^2 \cdot (n_{\lambda} + 2) \cdot 8 + \mathcal{M}[Bytes]$$
(3.5)

	approximate memory			
	requirement (Mb) for $n_{\lambda} =$			
$N_{v,max}$	11	9	7	5
2000	440	380	320	250
3000	930	800	660	520
4000	1630	1380	1140	890
5000	2520	2140	1760	1380
6000	3610	3060	2510	1960

Table 3.1: The LELUYA's memory requirements for various correlation matrix sizes  $N_{v,max}$  and the number of simultaneous wavelengths  $n_{\lambda}$  for  $\mathcal{M}=40Mb$ . The line shows the range of numbers where the HP Superdome at the UKY can be used (it has 2Gb of memory per processor).

where  $N_{v,max}$  is the maximum number of grid vertices used in the correlation matrix  $(N_{v,max}^2 \text{ is the size of this matrix})$  and  $n_{\lambda}$  is the maximum number of such matrices calculated simultaneously.  $\mathcal{M}$  is the rest of the memory requirement and it is about 70Mb for medium size grids and about 20Mb for small ones. The actual memory consumption varies during a single run, but this is the peak requirement that LELUYA needs. Since  $N_{v,max}$  can be just a subset of the total grid, we can adjust  $N_{v,max}$  and  $n_{\lambda}$  to fit the memory limitations of a particular machine. Table 3.1 shows an example of memory requirements suited for the HP Superdome at the University of Kentucky. In addition to this supercomputer, we also used a 65 Linux cluster KLAT2 at the Electrical Engineering Department.

The pre- and post-processing work during modeling, however, requires a single processor machine with access to visualization software. This includes the initial grid design and the final calculation of the theoretical images and spectra. We used various UNIX workstations at the Center for Computational Sciences, mostly a Pentium III (at 733MHz under Linux), a Silicon Graphics Octane (dual-processor at 270MHz each), and a Pentium 4 (at 2.4GHz under Linux). The majority of the code development has also been performed on these workstations. The visualization has been usually performed on one computer with a Pentium III (at 1.0GHz under MS Windows).

Visualization is an important component of our work, either as a code debugging tool

or for data output. A part of the LELUYA's output is in the form of the Virtual Reality Modeling Language (VRML) scripts that can be visualized in 3D with freeware browsers on various platforms. For this purpose, we used the SGI's Cosmoplayer (for IRIX) and Cortona by ParallelGraphics (for MS Windows). LELUYA can also provide the output in form of PovRay scripts. PovRay is an open source software for photo-realistic image rendering. In the future, our goal is to develop a special GUI for LELUYA which would remove dependence on other visualization tools and scripts/languages.

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## Chapter 4

# Bipolar outflow on the Asymptotic Giant Branch—the case of IRC+10011

#### Abstract<sup>(1)</sup>

Near-IR imaging of the AGB star IRC+10011 reveal the presence of a bipolar structure within the central ~ 0.1" of a spherical dusty wind. The density decreases as  $r^{-1/2}$ within an opening angle of ~ 30° about the bipolar axis, while outside, the wind displays the standard  $r^{-2}$  density profile. The image asymmetries originate from ~ 10<sup>-4</sup> M<sub> $\odot$ </sub> of swept-up wind material in an elongated cocoon. The cocoon confines bipolar jets that drive its expansion. This expansion started ~ 200 years ago, while the total lifetime of the circumstellar shell is ~ 4,000 years. Similar bipolar expansion, at various stages of evolution, has been recently observed in a number of other AGB stars, culminating in jet breakout from the confining spherical wind. The bipolar outflow is triggered at a late stage in the evolution of AGB winds, and IRC+10011 provides its earliest example thus far. These new developments enable us to identify the first instance of symmetry breaking in the evolution from AGB to planetary nebula.

<sup>&</sup>lt;sup>(1)</sup>The work described in this chapter was performed in collaboration with T. Blöcker, G. Weigelt, and K.-H. Hofmann from Max-Planck-Institut für Radioastronomie, Bonn, Germany. I would like to thank them for their hospitality during my multiple visits to the Institute, especially to Dr.Weigelt for his support and help.

## 4.1 Introduction

The transition from spherically symmetric Asymptotic Giant Branch (AGB) winds to non-spherical Planetary Nebulae (PNe) represents one of the most intriguing problems of stellar astrophysics. While most PNe show distinct deviations from spherical symmetry, their progenitors, the AGB stars, are conspicuous for the sphericity of their winds (see, e.g., review by Balick & Frank 2002). There have been suggestions, though, that deviations from sphericity may exist in some AGB winds, and perhaps could be even prevalent (Plez & Lambert 1994, Kahane at al. 1997). Thanks to progress in high resolution imaging, evidence of asymmetry has become more conclusive for several objects in recent years (V Hya: Plez & Lambert 1994, Sahai et al. 2003; X Her: Kahane & Jura 1996; IRC+10216: Skinner et al. 1998, Osterbart et al. 2000, Weigelt et al. 2002; RV Boo: Bergman et al. 2000, Biller et al. 2003; CIT6: Schmidt et al. 2002).

The star IRC+10011 (= IRAS 01037+1219, also known as CIT3 and WXPsc), an oxygen-rich long-period variable with a mean infrared variability period of 660 days (Le Bertre 1993), is one of the most extreme infrared AGB objects. This source served as the prototype for the first detailed models of AGB winds by Goldreich & Scoville (1976) and of the OH maser emission from OH/IR stars by Elitzur, Goldreich, & Scoville (1976). The optically thick dusty shell surrounding the star was formed by a large mass loss rate of  $\sim 10^{-5} \text{ M}_{\odot} \text{yr}^{-1}$ . The shell expansion velocity of  $\sim 20 \text{ km s}^{-1}$  has been measured in OH maser and CO lines. Various methods and measurements suggest a distance to IRC+10011 in the range of 500 to 800 pc

For an archetype of spherically symmetric AGB winds, the recent discovery by Hofmann et al. (2001; H01 hereafter) of distinct asymmetries in the IRC+10011 envelope came as a surprise. They obtained the first near infrared bispectrum speckle-interferometry observations of IRC+10011 in the J-, H- and K'-band with respective resolutions of 48 mas, 56 mas and 73 mas. While the H- and K'-band images appear almost spherically symmetric, the J-band shows a clear asymmetry. Two structures can be identified: a compact elliptical core and a fainter fan-like structure. Hofmann et al. also performed extensive one-dimensional radiative transfer modelling to explain the overall spectral energy distribution (SED) and angle-averaged visibility curves. Their model required a dust shell with optical depth  $\tau(0.55\mu m) = 30$  around a 2250 K star, with a dust condensation temperature of 900 K. This one-dimensional model successfully captured the essence of the circumstellar dusty environment of IRC+10011 but could not address the observed image asymmetry and its variation with wavelength. In addition, the model had difficulty explaining the far-IR flux, requiring an unusual transition from a  $1/r^2$  density profile to the flatter  $1/r^{1.5}$  for r larger than 20.5 dust condensation radii. Finally, the model produced scattered near-IR flux in excess of observations.

We report here the results of 2D radiative transfer modelling of IRC+10011 that successfully explain the observed asymmetries. After analyzing in §4.2 general observational implications we describe in §4.3 our model for a bipolar outflow in IRC+10011. In §4.4 we present detailed comparison of the model results with the data and resolution of the problems encountered by the 1D modelling. The discussion in §4.5 advances arguments for the role of bipolar jets in shaping the circumstellar envelope of IRC+10011 and other AGB stars. We conclude with a summary in §4.6.

## 4.2 Observational Implications

The near-IR images, especially the J-band, place strong constraints on the dust density distribution in the inner regions. Emission at the shortest wavelengths comes from the hottest dust regions. For condensation temperature ~ 1,000 K the peak emission is at ~  $4\mu$ m, declining rapidly toward shorter wavelengths. At 1.24  $\mu$ m, the J-band is dominated by dust scattering. It is easy to show that scattering by a  $1/r^p$  dust density distribution produces a  $1/r^{p+1}$  brightness profile. The J-band image from H01 is elongated and axially symmetric. Along the axis, the brightness declines from its central peak as  $1/r^3$  in one direction, corresponding to the  $1/r^2$  density profile typical of stellar winds. But in the other direction the brightness falls off only as  $1/r^{1.5}$ , corresponding to the flat, unusual  $1/r^{0.5}$  density profile.

The large scale structure is not as well constrained by imaging. However, all observations are consistent with the following simple picture: An optically thick spherical wind

has the standard  $1/r^2$  density profile. Since the buildup of optical depth is concentrated in the innermost regions for this density law, the near-IR imaging penetrates close to the dust condensation region. The wind contains an imbedded bipolar structure of limited radial extent and density profile  $1/r^{0.5}$ . The system is observed at an inclination from the axis so that the wind obscures the receding part of the bipolar structure, creating the observed asymmetry of the scattering image, which traces directly the density distribution. The inclination angle must be  $\leq 45^{\circ}$  since a larger value starts to expose the receding part. But the inclination cannot be too small because the approaching part would get in front of the wind hot dust, leading to a strong 10  $\mu$ m absorption feature, contrary to observations. Because of its shallow density profile, the column density of the bipolar structure *increases* as  $r^{1/2}$  away from the condensation cavity, and the size of J-band image corresponds to the distance where the scattering optical depth reaches unity. Regions further out do not show up because of self-absorption. Dust emission is affected also by the temperature distribution, and the central heating by the star tends to produce spherical isotherms. Images taken at longer wavelengths, such as the K-band, can thus appear more symmetric.

Some qualitative estimates of the gas density follow immediately. The wind optical depth at the J-band must be  $\geq 1$ . This optical depth is accumulated close to the dust condensation radius, roughly  $3 \times 10^{14}$  cm for a distance of 650 pc. Assuming a standard dust-to-gas ratio of 1:100, the gas density at the condensation radius is  $\geq 3 \times 10^7$  cm<sup>-3</sup>. For the bipolar structure, the J-band optical depth is  $\sim 1$  across the size of the observed image, which is  $\sim 2 \times 10^{15}$  cm. This leads to a density estimate of  $\sim 7 \times 10^6$  cm<sup>-3</sup> at the condensation radius within the bipolar structure. These rough estimates are within a factor 10 of the results of the detailed modelling described below.

The density at the base of the outflow is about an order of magnitude lower in the bipolar structure than in the wind region. An outflow can bore its way through another denser one only if its velocity is higher so that it plows its way thanks to its ram pressure. The propagation of such high-velocity bipolar outflows has been studied extensively in many contexts, beginning with jets in extragalactic radio sources (Scheuer 1974). The jet terminates in a shock, resulting in an expanding, elongated cocoon similar to the

observed bipolar structure. With a  $1/r^{1/2}$  density law, most of the bipolar structure mass is concentrated at its outer edge with the largest r, consistent with the structure of the expanding cocoon.

## 4.3 2D Model of IRC+10011

For our working model we adopt for the bipolar structure the geometry shown in figure 4.1, which requires the minimum number of free parameters. Each polar cone is described by its half-opening angle  $\theta_{\rm cone}$  and radial extent Apart from disconti- $R_{\rm cone}$ . nuities across the cone boundaries, the density depends only on r. It varies as  $1/r^{1/2}$  inside the cones and  $1/r^2$  outside, out to some final radius  $R_{\text{out}}$ . To complete the description of the geometry we need to specify its



Figure 4.1: Sketch of the 2D model for the circumstellar dusty shell around IRC+10011. In a spherical wind with the standard  $1/r^2$  density profile are imbedded two polar cones with half-opening angle  $\theta_{cone}$  and a  $1/r^{0.5}$  density profile. The system is viewed from angle i to the axis.

inner boundary, and it is important to note that this cannot be done a priori. Dust exists only where its temperature is below the condensation temperature  $T_c$ . Following H01 we select  $T_c = 900$  K. The dust inner boundary, corresponding to the radial distance of dust condensation,  $R_c$ , is determined from

$$T(R_{\rm c}(\theta)) = T_{\rm c} \tag{4.1}$$

The equilibrium dust temperature, T, is set by balancing its emission with the radiative heating. But the latter includes also the diffuse radiation, which is not known beforehand when the dust is optically thick; it can only be determined from the overall solution. Furthermore, because the spherical symmetry is broken by the cones, the shape of the dust condensation surface can be expected to deviate from spherical and is not known apriori. Therefore equation 4.1 completes the description of the geometry with an implicit definition of the inner boundary  $R_{\rm c}(\theta)$ .

The radiative transfer problem for radiatively heated dust possesses general scaling properties (Ivezic & Elitzur 1997). As a result,  $T_c$  is the only dimensional quantity that need be specified. All other properties can be expressed in dimensionless terms. Luminosity is irrelevant, the only relevant property of the stellar radiation is its spectral shape, which we take as black-body at  $T_{\star} = 2,250$  K. For individual dust grains, the only relevant properties are the spectral shapes of the absorption and scattering coefficients. For these we adopt spectral profiles corresponding to the silicate grains of Ossenkopf, Henning & Mathis (1992) with the standard size distribution described by Mathis, Rumpl & Nordsieck (1977; MRN). These properties are the same everywhere.

Density and distance scales do not enter individually, only indirectly through overall optical depth. With two independent density regions, the problem definition requires two independent optical depths. For this purpose we choose  $\tau_{\rm V}^{\rm a}$  and  $\tau_{\rm V}^{\rm e}$ , the overall optical depths at visual wavelengths along the axis and the equator, respectively. Spatial dimensions can be scaled with an arbitrary pre-defined distance, which we choose as the dust condensation radius in the equatorial plane,  $R_{\rm c}(90^{\circ})$ . The radial distance r is thus replaced by  $\rho = r/R_{\rm c}(90^{\circ})$  so that, e.g.,  $\rho_{out} = R_{\rm out}/R_{\rm c}(90^{\circ})$ . Equation 4.1 becomes an equation for the scaled boundary of the condensation cavity. The relation between angular displacement from the star  $\vartheta$  and the distance  $\rho$  is

$$\vartheta = \frac{\vartheta_{\star}}{2\rho_{\star}}\rho \tag{4.2}$$

where  $\vartheta_{\star}$  is the stellar angular size and  $\rho_{\star} = R_{\star}/R_{\rm c}(90^{\circ})$  is the scaled stellar radius. Physical dimensions can be set if one specifies a stellar luminosity  $L_{\star}$ , which determines the condensation radius  $R_{\rm c}(90^{\circ})$ .

To summarize, in all of our model calculations the following quantities were held fixed: grain properties,  $T_c = 900$  K and  $T_{\star} = 2,250$  K. In addition, we kept the outer boundary fixed at  $\rho_{out} = 1000$ . We varied  $\tau_{\rm V}^{\rm a}$ ,  $\tau_{\rm V}^{\rm e}$ ,  $\theta_{cone}$  and  $\rho_{cone}$ . Once a model is computed, comparison with observations introduces one more free parameter, the viewing angle i.

#### 4.3.1 Model calculations

We developed a new 2D radiative transfer code, LELUYA, that can handle arbitrary axially symmetric dust configurations without approximations. The dust scattering, absorption and thermal emission are solved exactly thanks to newly developed parallel algorithms, which will be described in a separate publication. The central source of radiation has a finite size instead of the often used point source approximation. In addition to the coupled equations of radiative transfer and temperature equilibrium, LELUYA solves equation 4.1 to determine the shape of the dust-free cavity around the central heating source. Another unique feature is a highly unstructured triangular self-adaptive grid that allows LELUYA to resolve simultaneously many orders of magnitude in both spatial and optical depth space. All grid points are coupled with each other through a correlation matrix based on the dust scat-



Figure 4.2: The computational grid. Top panel: Large scale view. Bottom panel: A zoom into the central region. Some radial dimensions of the dustfree cavity are listed in terms of the dust condensation distance in the equatorial plane. The stellar radius is  $\rho_{\star} = 0.153$ . Temperature is calculated at the grid points marked as spheres (their sizes carry no particular meaning).



Figure 4.3: Angular variation of  $\tau_{\rm V}$ , the optical depth at visual wavelengths along radial rays from the condensation boundary up to the indicated radius  $\rho$ . The input parameters specify  $\tau_{\rm V}(\theta = 0^\circ) = \tau_{\rm V}^{\rm a}$  and  $\tau_{\rm V}(\theta = 90^\circ) = \tau_{\rm V}^{\rm e}$  at  $\rho = \rho_{\rm out}$ .

tering. A simple matrix inversion gives the solution of radiative transfer for a given dust temperature distribution without any iterations. The temperature is then updated and the procedure repeated. Luminosity conservation within 5% is achieved in only three steps.

Figure 4.2 shows LELUYA's computational grid for the best fit model with  $\tau_{\rm V}^{\rm e} = 40$ ,  $\tau_{\rm V}^{\rm a} = 20$ ,  $\rho_{cone} = 700$ , and  $\theta_{cone} = 15^{\circ}$ . The upper panel shows a large scale view, the lower panel shows a zoom-in toward the central region. Three grids of different resolutions were created for three sets of wavelengths, based on the optical depth variation. The first grid has 2982 points and starts with  $\tau^{\rm e} = 120$  at  $0.2\mu$ m, the shortest wavelength considered; this is the grid shown in the figure. The second grid has 2836 points and starts at wavelengths with  $\tau^{\rm e} = 1.2$ . The third has 2177 grid points for wavelengths with  $\tau^{\rm e} \leq 0.1$ . Angular integration around a grid point is performed over a highly non-uniform self-adaptive angular grid (with about 550 rays on average).



Figure 4.4: Temperature distribution around the condensation cavity. The contours start at 850 K and decrease at 50 K intervals. The dust condensation temperature is 900 K.

The grid traces the dust density and optical depth variations. The condensation surface determined by LELUYA completes the definition of the geometry, and its irregular shape causes a variation of the optical depth along radial directions, shown in figure 4.3. The shape of the condensation cavity reflects the energy density of the local radiation field. Since the diffuse radiation in the cones is weaker than in the equatorial region, the dust there must get closer to the star to get heated to the same temperature. The condensation distance is reduced up to 13% on the axis in comparison to the equator. The stellar radius is  $\rho_{\star} = 0.153$ , that is, the condensation surface is ~ 6 stellar radii away from the stellar surface.



Figure 4.5: Radial temperature profiles. There are two distinct temperature regions, separated by  $\theta_{\text{cone}} = 15^{\circ}$  (see figure 4.4). The  $\theta > 15^{\circ}$  profile is hardly affected by the presence of the cones.

#### 4.3.2 2D Temperature Profile

Figure 4.4 shows the dust temperature distribution around the condensation cavity. Because of the central heating, the temperature decreases with radial distance and tends to create circularly symmetric isotherms, but the asymmetric diffuse radiation distorts them. There are two distinct temperature zones separated at  $\theta = \theta_{\text{cone}}$ . Within each zone the temperature is roughly dependent only on r. These radial temperature profiles are presented in Figure 4.5. In the wind region ( $\theta > \theta_{\text{cone}}$ ) the temperature is almost identical to an equivalent one-dimensional envelope without the cones. This result reflects the fact that the volume of the cones is relatively small.

#### 4.3.3 Luminosity Conservation

Luminosity conservation is the test determining convergence to the correct physical solution. A decrease in computed luminosity indicates energy sink due to insufficient spatial grid resolution, while an increase reflects energy excess due to a coarse angular grid. It is important to note that because of the lack of spherical symmetry, *the bolometric flux*  does vary over spherical surfaces. The conserved quantity is luminosity, the energy transmitted per unit time across any surface enclosing the star. For a sphere of radius  $\rho$ , the luminosity is computed from the radial component of the bolometric flux vector  $F_{\text{bol},r}$  via

$$L(\rho) = 4\pi\rho^2 \int_0^1 F_{\text{bol},r}(\rho,\theta) \, d\cos\theta.$$
(4.3)

The luminosity conservation relation is

$$\frac{L(\rho)}{L_{\star}} = 1 \qquad (4.4)$$

at every  $\rho$ , where  $L_{\star}$ is the stellar luminosity. Our model calculations conserve luminosity within 5% at all radii, as can be seen from figure 4.6.



Figure 4.6: The luminosity calculated over spherical surfaces of radius  $\rho$  (eq. 4.3), demonstrating conservation within the prescribed error tolerance of 5%.

In spherical symmetry  $F_{\text{bol},r}$  is  $\theta$ -independent and  $4\pi\rho^2 F_{\text{bol},r}/L_* = 1$ . When the spherical symmetry is broken  $F_{\text{bol},r}$  becomes  $\theta$ -dependent and  $4\pi\rho^2 F_{\text{bol},r}(\theta)/L_*$  can exceed unity in certain directions, corresponding to locally enhanced energy outflow. Figure 4.7 shows the angular variation of  $F_{\text{bol},r}(\theta)$  and its following five contributions: stellar, inward and outward emission, and inward and outward scattered flux. These angular variations are shown at  $\rho = 1.1$ , 500 and 1000. The small spikes in  $F_{\text{bol},r}$  close to  $\theta_{\text{cone}}$  are real, reflecting the irregular shape of the dust condensation surface. Even though these irregularities are spatially small, their effect on optical depth variations magnifies their importance. At small radii, energy outflow through the cones is enhanced in comparison with the wind and is the main reason for their higher temperature. This region is dominated by stellar contribution. At large radii these roles are reversed, the diffuse radiation (mostly dust emission) takes over and the temperatures inside and outside the cones become equal. Both behaviors are easily understood from the radial variation of optical depth shown in figure 4.3.



Figure 4.7: Angular dependence of the radial bolometric flux over spheres of radius  $\rho = 1.1$ , 500 and 1000. The numerical precision of luminosity conservation (eq. 4.4) is indicated from the listed  $L(\rho)/L_{\star}$  in each panel.
# 4.3.4 Radiation Pressure

Because of the flux variation on spherical surfaces, the radiation pressure force includes a tangential component in addition to the standard radial one. This force asymmetry traces the largest non-radial gradients of optical depth. Figure 4.8 shows the ratio between the tangential and radial components along the edge of a polar cone, where this ratio is the largest. The asymmetry is over 10% in the vicinity of the condensation cavity, pointing toward the cone where the density is lower. The tangential force diminishes fast with radial distance, disappearing already at  $\rho \sim 1.5$ . It reappears at larger radii, but is now less than few percents of the radial force and pointing away from the cone. A significant force asymmetry is present only close to the edge of cones and is negligible everywhere else. This can be seen in figure 4.9, which shows a map of the ratio of tangential to radial forces.



Figure 4.8: Radial dependence of the ratio between the tangential and radial components of the radiation pressure force along an angle of 16° from the axis. The drawing outlines the positive directions of the components.



Figure 4.9: Radiation pressure force asymmetry around the condensation cavity. Colors and contours show the value of the tangential to radial force ratio. The island of asymmetry points toward the cone, as seen in figure 4.8.



Figure 4.10: The model SED is shown with the thick, smooth solid line. Data (see H01) are indicated with various symbols and all other lines. The inset shows an expanded view of the  $10\mu m$  region.

# 4.4 Comparison with Observations

A detailed discussion of the data is available in H01. Our modelling procedure focused on fitting the SED and the visibility functions, leading to the best-fit model parameters listed in §4.3.1. The model SED is shown in figure 4.10. The  $10\mu$ m region is difficult to fit in all detail. Any further improvement would probably require more complicated geometry and/or modified dust properties. The SED is quite insensitive to changes in the inclination angle. The displayed model has  $i = 25^{\circ}$ , although there is no dramatic change up to  $i = 40^{\circ}$ . The near-IR images place much stronger constraints on the inclination angle.

The SED fit shows two major improvements over the 1D model fit of H01: (1) a much better fit to the near-IR, and (2) there is no need for the unusual  $1/r^{1.5}$  dust density profile in the stellar wind to fit the far-IR. While the rest of the envelope exhibits the standard  $1/r^2$  wind density profile, the cones are now the major source of far-IR flux,



Figure 4.11: Left: The model SED and its breakup to the stellar, dust scattering and emission components, as indicated. Right: Wavelength variation of the relative contribution of each component to total flux. Note the fast change from scattering to emission dominance around  $2\mu m$ . This transition is responsible for the observed wavelength variation of the image asymmetry in the near-IR.

emitting roughly twice as much as the rest of the envelope. Thus the far-IR flux becomes a measure of the total amount of mass in the cones, a point discussed further in §4.5.2.

The contributions of different components to the total flux are shown in the left panel of figure 4.11, with the fractional contributions shown in the right panel. The stellar component is reduced in comparison with the 1D model because of the larger optical depth toward the star. The scattering contribution is increased because of escape through the cone toward the observer. This "scattering hole" is the main source of the observed J-band image asymmetry. The fit yields a bolometric flux of  $F_{\rm bol} = 10^{-9} \,\mathrm{W/m^2}$ , corresponding to  $\vartheta_{\star} = 10.82$  mas for the stellar angular size, similar to the 10.9 mas derived in H01. Another approach to deriving  $\vartheta_{\star}$  would be from fitting of the images, but such fits produce much larger errors. The angular size of the dust condensation cavity is ~ 70 mas.

# 4.4.1 Visibility Functions and Images

With the model parameters set from the SED, the surface brightness distribution is fully determined, and the visibility functions are calculated from the brightness. For comparison with observations, the visibility must be normalized with the flux collected within  $\Theta_{\rm FV}$ , the instrumental field of view. If the image is divided into  $N \times N$  pixels then the



Figure 4.12: Visibility functions. Lines are model predictions, symbols are data points from H01 (near-IR) and Lipman et al. 2000 (11  $\mu$ m).

spatial frequency is  $q_i = i/\Theta_{\rm FV}$ , where i = 1...N. The results, shown in figure 4.12, contain no additional free parameters. In contrast with the SED, the visibility displays a strong sensitivity to the grain size. A change of only 0.05  $\mu$ m in the maximum grain size  $a_{\rm max}$  has a significant effect on the visibility curves. Our model has  $a_{max} = 0.20 \ \mu$ m, resulting in good fits for both the SED and the four different visibility curves.

The J-band visibility is the most difficult to model because it is dominated by the scattered light and thus very sensitive to fine details of the density distribution and grain size. Since the agreement between data and theory is better for small scales (higher spatial frequency), the quality of the fit to the J-band image can be expected to deteriorate with distance from the star. The model does not explain the puzzling drop in the H-band visibility at  $q \gtrsim 14$  cycles per arcsec, corresponding to structure smaller than the condensation cavity. Since a similar drop is not present in the J-band, it must correspond to material that emits but does not scatter light significantly. Hot gas might be a possible



Figure 4.13: Theoretical J-band  $(1.24\mu m)$ , H-band  $(1.65\mu m)$ , and K'-band  $(2.12\mu m)$  images of IRC+10011. Upper row: images for perfect resolution, without PSF convolution. The dot at the center of each image is the star. The nearby bright fan-shaped structure is scattered light escaping through the cone. Lower row: Images convolved with the instrumental PSF of H01. Contours are plotted from 1.5% to 29.5% of the peak brightness in steps of 1%. The transition from scattered light dominance in the J-band to thermal dust emission in the K'-band creates a sudden disappearance of the image asymmetry.

explanation.

Our model images and their convolution with the instrumental PSF of H01 are shown in figure 4.13. The comparison between the model and observed images is satisfactory, indicating that the overall geometry is properly captured by our simple model. The "halo" around the star in J-band model image is brighter than observed, indicating possible dust accumulation close to the equatorial region. The overall image asymmetry is much more prominent in the J-band, where dust scattering dominates the radiative transfer. As the wavelength shifts toward dominance of dust thermal emission, the image becomes more symmetric. The reason is that scattered light traces directly the density distribution while the dust emission is affected also by the temperature distribution. Because of the central heating, the isotherms tend to be spherical. The asymmetric dust absorption distorts these shapes, but the deviations from circularity are small, as is evident from figure 4.4, especially at the high dust temperatures traced by the K-band image. As a result, the image becomes more symmetric, especially after convolution with the PSF as shown in the lower panel of figure 4.13.



Figure 4.14: J-band brightness profiles along the major and minor axes. Thick lines show the model predictions with and without PSF convolution. The thin lines show the profiles from the H01 data above the noise level (within 1.5% of the peak brightness). The strong central peak in the theoretical profile is the star, while the secondary peak visible on the major axis is light scattered from the polar cone.

As evident from the figure, the PSF convolution smears out the star and the nearby fan-shaped structure into one broad elongated peak whose center is shifted from the stellar position. This shift is more clearly noticeable in the brightness profiles, shown in figures 4.14–4.16. The shift is 8.3 mas along the major axis in the J-band and 2.8 mas for the H- and K'-bands. The images provide tight constraints on the inclination angle. Neither  $i = 20^{\circ}$  nor  $i = 30^{\circ}$  produce acceptable fits, so that  $i = 25^\circ \pm 3^\circ.$ 

# 4.5 Discussion

Thanks to the scaling properties of dust radiative transfer, neither luminosity, distance or density absolute scales were specified. The distance to the source of  $650\pm150$  pc fixes those scales. The dust condensation radius is  $R_c(90^\circ) = 23 \pm 5$  AU, so that the wind extends to  $R_{\rm out} = 23,000$  AU and the luminosity is  $1.310^4 \,\mathrm{L}_{\odot}$ . With a wind velocity of 20 km s<sup>-1</sup>, its duration is 3,800 years.

# 4.5.1 Dust Properties

Our models employ silicate grains from Ossenkopf et al. (1992) with the standard MRN size distribution. We found that the upper limit on the grain sizes had to be reduced to  $a_{\rm max} = 0.20 \ \mu {\rm m}$  from the standard 0.25  $\mu$ m. While this change made little difference in the SED analysis, it was necessary for proper fits of the visibility curves. The most important effect of  $a_{\max}$  is control of the crossover from scattering to emission dominance, crucial for explanation of the observed change from elongated to circular images between the J-



Figure 4.15: *H-band brightness profiles, same as figure* 4.14.

and K-bands (see §4.4.1). Although we cannot claim to have determined the precise magnitude of  $a_{\text{max}}$ , the fact that it is smaller than the standard seems certain.

The dust properties in our model were the same everywhere to minimize the number

of free parameters. In a detailed study of the proto-planetary nebula IRAS 16342-3814, Dijkstra et al. (2003) find that the maximum grain size varies from  $\sim 1.3 \ \mu\text{m}$  in a torus around the star to  $\sim 0.09 \ \mu\text{m}$  in the bipolar lobes. If such a variation in dust properties can occur already on the AGB, the  $a_{\text{max}}$  we find would represent an average over the cones and wind regions.

## 4.5.2 Circumstellar Mass and its Distribution

The IR flux observations determine the total amount of emitting dust. Assuming a standard  $n_d \sigma_d/n = 10^{-21}$  cm<sup>2</sup>, the overall mass of the IRC+10011 circumstellar shell is 0.13 M<sub> $\odot$ </sub>. This copious amount of mass indicates that the star is close to the end of its AGB evolution. With 3,800 years as the duration of the current phase, the corresponding mass loss rate is  $\dot{M} = 3 \times 10^{-5}$  M<sub> $\odot$ </sub> yr<sup>-1</sup>.

Although IR fluxes provide a good measure of overall mass, they offer little guidance about its geometric distribution. The only tight con-



Figure 4.16: K-band brightness profiles, same as figure 4.14.

strains on the properties of the bipolar structure are imposed by the near-IR imaging and involve its innermost regions. From the brightness level at near-IR, the cones must extend at least up to  $\rho \sim 8$  and the optical depth across this region is  $\tau_V \sim 1.4$ . The corresponding gas density at the base of each cone is then  $n_{1c} = 1.3 \times 10^6$  cm<sup>-3</sup> and the mass the cones contain within the required distance is only  $\sim 2 \times 10^{-6}$  M<sub> $\odot$ </sub>. In contrast, the gas density at the base of the wind region (obtained from  $\tau_{\rm V}^{\rm e} = 40$ ) is  $n_{\rm 1w} = 1.7 \times 10^8$  cm<sup>-3</sup>. The large density disparity amplifies our earlier conclusion that the bipolar cones are sustained by high-velocity ram pressure.

The full extent of each cone remains uncertain, though, because the near-IR brightness drops below current detection capabilities at  $\rho \gtrsim 10$ . Our approach to the radiative transfer modelling was to employ the minimal geometry with the least number of free parameters that can still explain the observations, thus our model should be considered only a first-order approximation to the actual structure of IRC+10011. While the properties of the bipolar structure in the innermost regions can be considered secure, it can be shown that the cones cannot be as large as derived from our simple approach. If they indeed extended all the way to  $\rho_{\rm cone} = 700$ , as required by our model fit to the SED, the ratio of mass contained in the two cones and in the wind region would be  $M_{\rm cone}/M_{\rm wind} =$ 1.7, that is, most of the circumstellar mass is in the cones. Since the fractional volume occupied by the cones is only 0.034, such large mass could not be swept-up wind material. However, building it up with enhanced mass flux through the polar regions runs into similar problems. Mass conservation along stream lines yields  $v_1 t = R_1 \int \eta \rho^2 d\rho$ , where  $v_1$ and  $n_1$  are the velocity and density at the streamline base  $R_1$ , t is the duration of the outflow and  $\eta(\rho) = n(\rho)/n_1$  is the dimensionless density profile. Applying this relation to streamlines in the cone and wind regions yields

$$\frac{v_1 t}{R_1}|_{\text{cone}} = \frac{2}{5} \rho_{\text{cone}}^{5/2}, \qquad \frac{v_1 t}{R_1}|_{\text{wind}} = \rho_{\text{out}}$$
(4.5)

Our model gives for the product  $v_1t/R_1$  a value of  $5.2 \times 10^6$  in the cone regions if  $\rho_{\rm cone} =$ 700 while in the wind this product is only 1000. Since the wind starts with a sonic velocity  $v_{1w} \sim 1 \text{ km s}^{-1}$ , the conical outflow would have to start with velocity  $v_{1c} \simeq 5.2 \times 10^3 t_w/t_c$ km s<sup>-1</sup>, where  $t_w$  and  $t_c$  are the wind and cones lifetimes. This is impossible since the bipolar structure would extend much further than the wind even for  $t_c = t_w$ ; taking a physical  $t_c \ll t_w$  only makes things worse. Furthermore, this argument can be easily extended to show that, irrespective of the magnitude of  $\rho_{\rm cone}$ , the mass in the cones could not be deposited purely by recent enhancement of polar mass loss rates. A substantial fraction, perhaps even all, of this mass must be swept-up wind material. This analysis shows that  $\rho_{\text{cone}}$  cannot be as large as required by our simple model. If  $\rho_{\text{cone}} \leq 100$ , our model would have to be further modified to account for the far-IR flux produced by the large mass removed from the cones. This mass can be placed elsewhere as long as its temperature distribution corresponds to far-IR wavelengths. The only self-consistent geometry to accomplish that is a toroidal configuration at distances of  $\geq 10^2$  AU. Indeed, 8.55  $\mu$ m imaging observations with spatial resolution of  $\rho \sim 50$  by Marengo et al. (1999) support this possibility. These observations indicate a probable extension along an axis almost perpendicular to the symmetry axis of the bipolar structure.

## 4.5.3 Jet Model for the Bipolar Structure

The small density at the base of the cones shows that their material has been evacuated and deposited at larger distances by a recent event. We propose the following simple scenario for the bipolar structure: High-velocity low-density jets were recently turned on at the polar regions. The jets cleared out polar cavities but are trapped by the material pushed ahead by their ram pressure, resulting in an expanding cocoon as described first by Scheuer (1974). Our model cones are a description of the current density distribution of the cocoon, a snapshot of an inherently dynamic structure. In this picture, the mass in the cones is swept-up ambient wind material and the cone boundary is then

$$\rho_{\rm cone} = \left(\frac{5}{2} \frac{n_{\rm 1w}}{n_{\rm 1c}}\right)^{2/3} = 47,\tag{4.6}$$

in agreement with the value implied by the Marengo et al. observations. The swept-up mass is only  $\sim 10^{-4} \,\mathrm{M_{\odot}}$ . The leading edge of the cocoon moves at velocity  $v_{\rm c} = \beta v_{\rm w}$ , where  $v_{\rm w}$  is the local wind velocity and  $\beta > 1$ . From pressure balance during jet confinement,

$$n_{\rm c}(v_{\rm c} - v_{\rm w})^2 = n_{\rm w} v_{\rm t}^2 \tag{4.7}$$

where  $n_{\rm c}$  and  $n_{\rm w}$  are densities across the cocoon leading edge and  $v_{\rm t}$  is the local speed of sound in the wind. This condition requires that the density of the cones be smaller than the ambient density into which they are expanding, i.e.,  $n_{\rm c} < n_{\rm w}$ , restricting the cone radial extension to  $\rho \leq 26$  which is slightly smaller than the derived  $\rho_{\rm cone}$ . We attribute this discrepancy to the approximate nature of our model in which the complex structure of the cocoon-wind boundary is replaced with the sharp-cutoff of the simple power-law density distribution of the cones. Taking  $n_c \simeq n_w$  at the cone boundary, pressure balance implies  $v_c \simeq v_w$ , consistent with a recent start of the jet confinement. Assuming that the cocoon radial boundary moves according to  $\rho_{\text{cone}} \propto t^{\alpha}$ , with  $\alpha \gtrsim 1$  to ensure acceleration, its velocity is  $v_c = \alpha \rho_{\text{cone}} R_1/t$ . This yields an estimate for the jet lifetime

$$t_{\rm jet} = \frac{\alpha}{\beta} \frac{R_1}{v_{\rm w}} \rho_{\rm cone} \simeq 200 \text{ years}$$
(4.8)

for  $\alpha/\beta \simeq 1$ .

Because of the steep decline of the wind density, the expansion accelerates rapidly as the cocoon boundary reaches lower density regions. Eventually it will break out of the wind, exposing the underlying jets. Indeed, a striking example of such a configuration comes from the recent observations, including proper motion measurements, of water masers in W43A by Imai et al. (2002). The observations reveal tightly collimated velocities of ~ 150 km s<sup>-1</sup> at distances up to ~ 0.3 pc at the two ends of an axis through the star. These masers are created by the impact of the jets on clumps in the surrounding medium. In addition to these far-away high-velocity masers, the source displays the usual configuration typical of OH/IR stars – OH and water masers in shells expanding with velocities ~ 9 km s<sup>-1</sup> with radii of ~ 500 AU. Therefore this source displays both the spherical AGB wind and the jets that broke through it.

### 4.5.4 Asymmetry Evolution in AGB Stars

IRC+10011 and W43A can be considered, respectively, the youngest and most evolved examples of sources displaying the evolution of bipolar jets working their way through AGB winds. The prototype C-rich star IRC+10216 shows circular shape on the 20" scale both in V-band (de Laverney 2003) and molecular line images (e.g., Dayal & Bieging 1995). But high-resolution IR imaging at the 0.1" scale reveal elongated structure similar to that in IRC+10011 (Osterbart et al. 2000, Weigelt et al. 2002). Unlike IRC+10011, though, where only the J-band image gives clear indication of asymmetry, in IRC+10216 it is evident even in the K-band. This strongly suggests that IRC+10216 represents a more advanced stage than IRC+10011 of the evolution of a jet-driven cocoon confined by the ambient spherical wind.

The C-rich star V Hya provides an example that is further along in evolution. Recent CO observations by Sahai et al. (2003) show that the bulk of the emission comes from an elongated structure centered on the star. In addition, two emission blobs are found at the opposite ends of an axis perpendicular to this elongation, one blue- the other red-shifted with velocities of 100–150 km s<sup>-1</sup>. This is the expected morphology of a bipolar outflow breaking from the confinement of the high-density region of the AGB wind. A similar structure has been found in the O-rich star X Her. Partially resolved CO observations by Kahane & Jura 1996 reveal a spherical component expanding with only 2.5 km s<sup>-1</sup> and two symmetrically displaced 10 km s<sup>-1</sup> components, likely to be the red and blue shifted cones of a weakly collimated bipolar flow. The bipolar lobes are ~ 1.5 times bigger than the spherical component. Finally, the C-rich star CIT6 presents an even more evolved system. A bipolar asymmetry dominates the image both in molecular line mapping by Lindqvist et al. (2000) and in HST-NICMOS imaging by Schmidt et al. (2002).

# 4.6 Summary and Conclusions

We find that the circumstellar shell of IRC+10011 contains about 0.13 M<sub> $\odot$ </sub>, extends to a radial distance of ~ 23,000 AU (~ 35") from the star and is ~ 3,800 years old. Roughly half of the circumstellar mass is concentrated in a toroidal structure whose size is  $\geq$  1,200 AU (~ 2"). The near-IR image asymmetries discovered within the central ~ 0.1" of this system originate from ~ 10<sup>-4</sup> M<sub> $\odot$ </sub> of swept-up wind material in a cocoon elongated along the axis, extending to a radial distance of ~ 1,200 AU. The cocoon expansion is driven by bipolar jets that it confines and that were switched on ~ 200 years ago. The axial symmetry of the J-band image eliminates the possibility of a companion star, unless closer than ~ 5 stellar radii. Higher sensitivity and/or better angular resolution would uncover image asymmetry in the K-band too.

Jet-driven cocoon expansion at various stages of development has now been observed in a number of AGB stars, culminating in breakout from the confining spherical wind (§4.5.4). The immediate post-AGB stage is believed to be the proto-planetary-nebula (PPN) phase. Indeed, jets are found to be quite common in PPN as shown by the recent observations of K3-35 (Miranda et al. 2001) and Hen 3-1475 (Riera et al. 2003), for example. The case of K3-35 is particularly striking because of its great similarity to the AGB star W43A: water masers at the tips of bipolar jets at a large distance from the systemic center, which is surrounded by masers in the standard spherical shell configuration. This strongly suggests that W43A provides a glimpse of the immediate precursor of K3-35.

These new developments enable us to identify the first instance of symmetry breaking in the evolution from AGB to planetary nebula. Bipolar asymmetry appears during the final stages of AGB mass outflow. Mounting evidence suggests that this asymmetry is driven by collimated outflow in the polar regions. More complex geometries emerge in the post-AGB phase from a mixture of various processes that could involve multiple jets, fast winds, etc. These processes operate in the environment shaped by the AGB phase, leading to the myriad of complex structures found in PPN sources (e.g. Su, Hrivnak & Kwok 2001).

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#### **REFEREED JOURNAL PUBLICATIONS:**

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