Master thesis

Ignace Bossuyt

2019-2020

Contents

Ι	Questions	5
1	Questions for professor Sundqvist	5
2	Questions for professor Samaey	6
3	Solved questions	7
4	Interesting problems	8
II	Monte Carlo Radiative Transfer	9
5	Glossary	9
6	General equations - first year overview	10
7	Very broad introduction & Summary 7.1 Definitions and equations	11 11 14
8	Introduction: course material (Sundqvist - CMPAA course) 8.1 EXERCISES: Introduction to numerical methods for radiation in astrophysics	15 15 17 17 17
9	The mathematics of Radiative Transfer 9.1 Auxiliary mathematics	18 18 18
10	Monte Carlo and Radiative Transfer (Puls)	19
	10.1 basic definitions and facts 10.2 about random numbers 10.3 MC integration 10.4 MC simulation 10.5 Exercise 1: RNG 10.6 Exercise 2: Planck-function 10.7 limb darkening	19 19 19 19 19 19

11 Introduction to Monte Carlo Radiation Transfer (Wood+) 11.1 Elementary principles	20 20 20 20 22 23
12 Challenges in Radiative Transfer (Ivan Milic) 12.1 Overview of the problem	24 24 24
13 Asymptotic Preserving Monte Carlo methods for transport equations in the diffusive limit (Dimarco+2018)	25
14 Splitting methods 14.1 Exercises	26 26
III Practical work and Exercises	27
15 Overview of exercises (PART I)	27
16 Overview of exercises (PART II)	27
17 Limb darkening	28
18 Investigation of program: pcyg.f90 18.1 Overview of variables	
19 Milic Exercises 19.1 Lecture 7	40 40
20 Mass loss from inhomogeneous hot star winds (Sundqvist)	41
21 Asymptotic preserving Monte Carlo methods for radiative transfer equation in diffusion limit (Dimarco+ 2018) 21.1 Goldstein-Taylor	42
IV Equation meetings	43
22 Meeting of 10 April 2019	43
23 Meeting of 17 April 2019	43
24 Meeting of 14 August 2019	43
V Thesis meetings	45
25 Meeting on 6 September 2019	45

Exercises, part II Via this link, you can go back to the exercises overview: Section 16.

Part I

Questions

1 Questions for professor Sundqvist

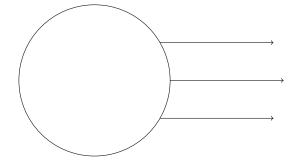
- \bullet book $Stellar\ Atmospheres$ [Mihalas].
- \bullet (for which star are the exerpimental data and what assumptions are used in the theory?)

Questions for professor Samaey

• what is the difference between Monte Carlo and equation-free computing?

3 Solved questions

- Sundqvist+ 2009: what is thermal velocity (see Wikipedia)
- Sundqvist+ 2009: what is line force (see explanation Dylan)
- unclassified: what is a flux limiter? (see course notes)
- unclassified: what is cross section of scattering (see Wikipedia)
- Puls manual: p.26: how does the Milne equation appear? (see library book)
- pcyg.f90: what are p-rays? (see anwser professor Sundqvist)
 - parallel rays leaving the atmosphere (of, e.g. a star)



- pcyg.f90: what is meant by Eddington limb-darkening? (see answer professor Sundqvist)
 - standard limb darkening
- Sundqvist+ 2009: what is the geometry of a slice?
- CMFAA course notes p.13 (the example) what is understood by plane-parallel geometry and is it 1D or 2D? (see answer professor Sundqvist)

• CMFAA course notes p.15: why is this called diffusion $F = T^3 \frac{dT}{dx}$ (flux proportional to local gradient in temperature)?

- unclassified: what is the terminal velocity v_{∞} ?
- unclassified: what is Sobo-distribution? (Sobolev distribution)
- pcyg.f90: for test_number = 2, why do we call it isotropic since isotropy of mu does not imply isotropy of theta? (myself, see definition of intensity)

84 Interesting problems

• inverse radiative transfer problem

Part II

Monte Carlo Radiative Transfer

5 Glossary

• SED: spectral energy distribution

• (spectral) line-force: force on material in stellar atmosphere

• LASER: Light Amplification by Stimulated Emission of Radiation

6 General equations - first year overview

6.0.1 Hydrodynamics

Euler equations, together with closing relation (e.g. ideal gas law).

primitive variables			
mass density	velocity	gas energy density	gas pressure
ρ	v	e	p

6.0.2 Radiation

Radiative transfer equation: intensity along a ray while interacting with medium. Photons are massless.

$$\left[\frac{1}{c}\partial_t + \vec{n}.\vec{\nabla}\right]I_{\nu} = \eta_{\nu} - \chi_{\nu}I_{\nu} \tag{1}$$

frequency	intensity	emissivity	total absorption
ν	$I_{ u}$	$\eta_ u$	$\chi_ u$

These deliver two equations

• the radiative energy equation (diffusion flux \vec{F}

$$\frac{\partial E}{\partial t} + \vec{\nabla} \cdot \vec{F} = \iint ... d\nu d\Omega \tag{2}$$

• radiative momentum equation

$$\frac{d\vec{F}}{\partial t} = \iint ... \vec{n} d\nu d\Omega \tag{3}$$

(after **integrating over all frequencies**). Depending on the geometry simplifications, one can e.g. integrate over all solid angles.

6.0.3 Radiation-Hydrodynamics

Combination delivers integral-diffusion equation

$$\frac{dI}{d\tau} = S - I$$

$$= \int I d\Omega - I$$
(4)

6.0.4 Challenges

- combination with hydrodynamics
- current analysis: simplified geometries (symmetry). E.g. in 2D, an ADI method is used and now also a multigrid method.
- \bullet complex geometry difficult to show in ray-tracing scheme
- steady-state vs. time dependent
- ullet focus on radiation equations

7 Very broad introduction & Summary

The material here originates from the master thesis of Nicolas Moens [Moe18] and from the course notes Introduction to numerical methods for radiation in astrophysics from professor Sundqvist.

7.1 Definitions and equations

7.1.1 Radiation equations

Specific intensity $I(s, \lambda, x, y, t)$

- restrict oursevels to time-independent, one-dimensional (1D) case $I(s, \theta, \lambda)$ where s is the direction of the light ray
- it satisfies Radiation Transfer Equation (RTE) $\boxed{\frac{dI_{\lambda}}{d\tau_{\lambda}} = S_{\lambda} I_{\lambda}}$
- with 'formal' solution $I(\lambda, \tau_{\lambda}) = I_0(\lambda) e^{-\tau_{\lambda}} \int_0^{\tau_{\lambda}} S(t) e^{-t} dt$
 - no emissivity S = 0 then $I(\lambda)I_0(\lambda)e^{-\tau_{\lambda}}$
 - no opacity then $I_0(\lambda) = \int_0^s \eta_{\lambda}(s) ds$
 - constant source function $I(\lambda, \tau) = I_0(\lambda)e^{-\tau_{\lambda}} + S(1 e^{-\tau_{\lambda}})$
 - if $S = a + b\tau$ then $I(\lambda) = a + \frac{b}{k_{\lambda}}$ with k_{λ} the opacity. A jump in opacity leads to the jump in intensity of the opposite sign.

7.1.2 RHD equations

The full RHD equations consist of

- five partial differential equations
- one HD closure equation, e.g. (i) variable Eddington tensor method or (ii) flux limited diffusion

Heat flux The heat flow rate density $\vec{\phi}$ satisfies the Fourier law $\vec{\phi} = -k\nabla T$. More information can be found for instance on [Wik18].

Specific intensity and its angular moments

specific intensity	$\Delta \epsilon = \boxed{I_{\nu}} A_1 A_2 / r^2 \Delta \nu \Delta t$
energy density	$E = \frac{1}{c} \iint I_{\nu} d\nu d\Omega$
flux vector	$F = \iint I_{\nu} n d\nu d\Omega$
pressure tensor	$P = \iint I_{\nu} nn d\nu d\Omega$
mean intensity	$J_{\nu} = \frac{c}{4\pi} E_{\nu}$
Eddington flux	$H_{\nu} = \frac{1}{4\pi} F_{\nu}$
Eddington's K	$K_{\nu} = \frac{c}{4\pi} P_{\nu}$

Eddington factor In general, the Eddington factor is a tensor, for 1D systems it is reduced to a scalar.

$$f_{\nu} = \frac{K_{\nu}}{J_{\nu}} = \frac{P_{\nu}}{E_{\nu}} \tag{5}$$

- isotropic radiation field
- radiation field stronly peaked in radial (i.e. vertical in cartesian) direction

7.1.3 Radiation transport equations, diffusion, equilibrium

- black body radiation (Planck function $I_{\nu} = J_{\nu} = B_{\nu}$)
- in general, extinction(absorption, scattering) and emission

$$\frac{dI_{\nu}}{ds} = j_{\nu} - k_{\nu}I_{\nu} \tag{6}$$

- Cartesian coordinates:

$$\frac{\partial I_{n,\nu}}{\partial t} \frac{1}{c} + n \nabla I_{n,\nu} = j_{\nu} - k_{n,\nu} I_{n,\nu}$$
(7)

- spherical coordinates
- 1D-problem with only variation along z-axis $\mu \frac{dI}{dz} = j kI$
- spherical symmetry $\mu \frac{\partial I}{\partial r} + \frac{1-\mu^2}{r} \frac{\partial I}{\partial \mu} = j kI$
- plane-parallel approximation

$$\mu \frac{dI}{dr} = j - kI \tag{8}$$

The angle μ is constant throughout the computational domain. Dividing by k_{ν} , this yields

$$\mu \frac{dI}{k_{\nu}dr} = \mu \frac{dI}{k_{\nu}dz} = S - I \tag{9}$$

- Oth moment equation: integrate Equation (7) over ν and Ω , i.e. $\int d\nu d\Omega$. Conservation of energy
- first multiply Equation (7) with $\frac{n}{c}$ and then do integration

7.1.4 Radiative Diffusion Approximation

The radiative diffusion approximation bridges two regimes: regimes with ...

- ullet on one hand, large optical depth $au\gg 1$: diffusion equation: temperature structure in a static stellar atmosphere
- on the other hand, where radiative transport is important

The diffusive approximation is the following: replace I = B or $I_{\nu} = B_{\nu}$.

$$I_{\nu} = B_{\nu} - \mu \frac{dB_{\nu}}{k_{\nu}dz} \tag{10}$$

This equation can be derived as a random walk of photons!

7.1.5 Applications and approximations for radiative forces

- definition of general radiative acceleration vector $g=\frac{1}{\rho c}\int\int nk_{\nu}I_{\nu}d\Omega d\nu$
 - $-\,$ continuum Thomson scattering
 - spectral line with extinction
 - * furthermore assume central continuum source

* then
$$g_{line} = \frac{F_{\nu}^0 k_L}{\rho c}$$

- ullet Sobolev approximation
- CAK theory

7.1.6 Optical depth (recap)

Optical depth: physical understanding Optical depth is the ratio of incident radiant power to transmitted radiant power ([WikiOpticalDepth]).

optical depth	optical depth along ray	line optical depth	Sobolev optical depth
$d\tau = k_{\nu}ds = \sigma_{nu}nds = \kappa \rho ds$	$\tau_{\mu,\nu} = \int_{z}^{z_{max}} \frac{\alpha_{nu}(z')}{\mu} dz' = \frac{\tau_{\nu}(z)}{\mu}$	$\tau_{\nu} = \int k_L \phi_{\nu} dl = \int \kappa \rho ds$	
$\tau_{\nu} = \int k_{\nu} ds = \int \sigma_{\nu} n ds$			•

with

- \bullet σ cross-section
- \bullet *n* number density
- κ mass absorption density
- ρ mass density
- k_{ν} extinction coefficient

7.2 Overview of symmetry assumptions

plane-parallel	1D atmosphere	
	bounded by horizontal surfaces	

8 Introduction: course material (Sundqvist - CMPAA course)

8.1 EXERCISES: Introduction to numerical methods for radiation in astrophysics

- 1. introduction
- 2. radiation quantities
 - exercise p.3:
 - on one hand, we know that $\Delta \epsilon \sim C/r^2$
 - on the other hand, from the definition we know that $\Delta \epsilon = I_{\nu} A_1 A_2 / r^2 \Delta \nu \Delta t$
 - combining these equations shows that I_{ν} is independent from r
 - exercise p.4:

_

• exercise 1:

$$-F_x = \int_0^\pi \left[I_\nu(\theta) \sin^2(\theta) \int_0^{2\pi} \cos(\phi) \right] d\theta d\phi = 0$$

- the same reasoning for $F_y = 0$
- exercise 2:
 - the equation follows from $d\mu = d\cos(\theta) = \sin(\theta)d\theta$
- exercise 3:
 - isotropic radiation field (i.e. $I(\mu) = I$) then we have $F_{\nu} = 2\pi \int_{-1}^{1} I \mu d\mu = 2\pi I \left. \frac{x^2}{2} \right|_{1}^{1} = 0$
- exercise 4

$$-F_{\nu} = 2\pi \int_{-1}^{1} I(\mu)\mu d\mu = 2\pi \int_{-1}^{0} I_{\nu}^{-} \mu d\mu + 2\pi \int_{0}^{1} I_{\nu}^{+} \mu d\mu = 2\pi I_{\nu}^{+}$$

- exercise p.7:
 - isotropic radiation field:
 - * although the radiation pressure is a tensor, we will denote it as a scalar $P_{\nu} = \frac{4\pi I_{\nu}}{c}$
 - * the radiation energy density $E_{\nu} = \frac{12\pi I_{\nu}}{c}$
 - * thus $f_{\nu} = \frac{1}{3}$
 - very strongly peaked in radial direction (beam): $I_{\nu} = I_0 \delta(\mu \mu_0)$ with $\mu_0 = 1$
 - * pressure tensor $P_{nu} = \frac{1}{c} \int I_0 \delta(\mu \mu_0) nn d\Omega$
 - * energy density $E_{\nu} = \frac{1}{c} \int I_{\nu} d\Omega$
 - * in this case $P_{\nu} = E_{\nu}$ thus $f_{\nu} = 1$
- 3. radiation transport vs. diffusion vs. equilibrium
 - exercise p. 12: 1D, Cartesian geometry, plane-parallel, frequency-independent and isotropic emission/extinction
 - radiation energy equation
 - * The equation follows by integrating Equation (8)
 - * By definition, $E = \frac{1}{c} \iint I_{\nu} d\nu d\Omega$
 - * thus $\frac{dE}{dr} = \int (j kI) d\nu d\Omega$ thus $\frac{dE}{dr} = \frac{(j kI) 4\pi (\nu_1 \nu_0)}{c}$

- * work out the integral taking into account frequency-independent and isotropic coefficients:
- zeroth momentum equations
 - * One must also take into account the specific form of the flux vector

$$F = \iint I_{\nu} n d\nu d\Omega = 2\pi \int_{-1}^{1} I_{\nu}(\mu) \mu d\mu$$

* thus
$$\frac{dF}{dr} = \frac{1}{c} \int (j-kI) n d\nu d\Omega$$
 thus $dF = \frac{(j-kI) 4\pi (\nu_1 - \nu_0) n}{c}$

- first moment equation
 - * similar reasoning

*
$$\frac{dP}{dr} = \int (j - kI)n \cdot n d\nu d\Omega$$
 thus $\left[\frac{dF}{dr} = \frac{(j - kI)4\pi(\nu_1 - \nu_0)n}{c}\right]$

• first exercise p. 15

$$-P = \frac{1}{c} \iint I_{\nu} \mu^{2} d\Omega d\nu = \frac{2\pi}{c} \int_{\nu} \int_{-1}^{1} I_{\nu} \mu^{2} d\mu d\nu = \frac{4\pi}{3c} \int B_{\nu} d\nu = \frac{aT^{4}}{3} = \frac{E}{3}$$

- second exercise p.15
 - assuming the diffusion limit,
 - flux-weighted mean opacity $\kappa_F = \frac{\int F_\nu \kappa_\nu d\nu}{\int F_\nu d\nu}$
 - Rosseland mean opacity $\frac{1}{\kappa_R} = \frac{\int_0^\infty \frac{1}{\kappa_\nu} \frac{dB_\nu}{dT}}{\int_0^\infty \frac{dB_\nu}{dT} d\nu}.$
 - * in the diffusion limit, $F_{\nu}=-\frac{4\pi}{3}\frac{dB_{\nu}}{k..dz}$ thus $\frac{dB_{nu}}{dT}=$
- third exercise p.15
- 4. the equations of radiation-hydrodynamics
- 5. numerical techniques for the radiative diffusion approximation
- 6. applications and approximations for a dynamically important radiative force in supersonic flows

• exercise p.27:
$$L_{SOB}=\Delta r=\frac{v_{th}}{dv/dr}=\frac{10[km/s]}{1000[km/s]/R_*}=0.01R_*$$

- 7. Appendix A: properties of equilibrium black-body radiation
 - exercise p. 29
 - this should be satisfied: $B_{\nu}d\nu = -B_{\lambda}d\lambda$ and also $\nu = \frac{c}{\lambda}$

- this is equivalent to saying that
$$0 = \nu d\lambda + \lambda d\nu$$
 or $d\lambda = -\frac{\lambda}{\nu} d\nu$ thus $B_{\lambda} = \frac{\nu}{\lambda} B_{\nu}$
- $B_{\lambda}(T) = \frac{\nu}{\lambda} \frac{2h\nu^{3}}{(\lambda\nu)^{2}} \frac{1}{e^{hc/\lambda kT} - 1} = \frac{2h\nu^{2}}{\lambda^{3}} \frac{1}{e^{hc/\lambda kT} - 1} = \frac{2hc^{2}}{\lambda^{5}} \frac{1}{e^{hc/\lambda kT} - 1}$

- first exercise p.31
 - derive that $\lambda_{max}T = 2897.8[\mu mK]$
- second exercise p.31
 - this is about the spectra of (unknown) stars
- first exercise p.32
 - see exercise 7
- second exercise p.32

September 17, 2019

17

- BB radiation: $I_{\nu} = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kt} 1}$
- the radiative flux for isotropic BB radiation is zero. See also exercise 3. This dus also holds for BB radiation.
- exercise p. 33
 - HR-diagram
- 8. Appendix B: Simple examples to the radiative transfer equation
 - first exercise p. 34
 - start from radiative transport equation $\mu \frac{dI}{ds} = \alpha \eta I$ in which $\eta = 0$ thus $\mu \frac{dI}{ds} = \alpha$
 - solving the ODE in the general case that $\alpha(s)$ is not constant:
 - * integrate the equation $\mu I = \int_0^D \alpha ds$
 - * ...
 - second exercise p. 34
 - * case $\tau(D) >> 1$: then $I(D) \approx S$
 - * case $\tau(D) << 1$: then $I(D) \approx I(0) + S(1-1) = I(0)$
 - first exercise p.35
 - * is the plane-parallel approximation valid for the solar photosphere?
 - second exercise p.35
 - * goal: find a solution to the equation $\mu \frac{dI_{\nu}}{d\tau_{\nu}} = I_{\nu} S_{\nu}$ where $I(\tau, \mu)$
 - * solution
 - \bullet second exercise p.35
- 9. Appendix C: connecting random walk of photons with radiative diffusion model
 - exercise p. 38. Computing the average photon mean-free path inside the Sun. $l=\frac{1}{\kappa\rho}=\frac{V_o}{\kappa M_o}[cm]$
 - exercise p.39. Computing the random-walk time (diffusion time) for photons

8.2 Implicit 1D solver (20-11-2018)

See computer code

8.3 ADI 2D Solver

See computer code

8.4 Area of a circle

See computer code

8.5 Limb Darkening

See Section 17.

9 The mathematics of Radiative Transfer

The material in this section is based on the book [Bus60].

9.1 Auxiliary mathematics

- $\cos(\Theta) = \cos(\theta)\cos(\theta') + \sin(\theta)\sin(\theta')\cos(\phi \phi')$
- phase function $p(\mu, \phi, \mu', \phi', \tau) = \sum_{n=0}^{N} \omega_n P_n(\cos(\Theta))$
 - isotropic scattering $p(\tau) = \omega_0(\tau)$
- equation of transfer $\boxed{\mu \frac{\partial I(\tau, \mu, \phi)}{\partial \tau} = I(\tau, \mu, \phi) \mathcal{S}(\tau, \mu, \phi)}$ with $\mathcal{S}(\tau, \mu, \phi) = B_1(\tau) + \frac{1}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} I(\tau, \mu', \phi') p(\mu, \phi, \mu', \phi') d\phi'$
 - axially symmetric with isotropic scattering $\mathcal{S}(\tau) = \frac{\omega_0(\tau)}{2} \int_{-1}^1 I(\tau,\mu') d\mu' = B_1(\tau) + \frac{\omega_0(\tau)}{2} \int_0^{\tau_1} \mathcal{S}(t) E_1(|t-\tau|) dt$
 - the Milne equation of the problem $(1 \omega_0 \bar{\Lambda})$ { mahtcalS(t)} = $B(\tau)$
 - * solve for S(t)
 - * then find $I(\tau, \mu)$

9.2 The H-functions

• characteristic equation

10 Monte Carlo and Radiative Transfer (Puls)

- 10.1 basic definitions and facts
- 10.2 about random numbers
- 10.3 MC integration
- 10.4 MC simulation

Radiative transfer in stellar atmospheres

- GOAL: spatial radiation energy density $E(\tau)$ in an atmospheric layer
 - only photon-electron scattering
 - $-\tau$ is the optical depth
- Milne's integral equation $E(\tau) = \frac{1}{2} \int_0^\infty E(t) E_1(|t-\tau|) dt$
 - analytical solution $\frac{E(\tau)}{E(0)} = \sqrt{3}(\tau + q(\tau))$
 - MC simulation
 - * emission angle
 - * optical depth until next scattering event
 - * scattering angle
- HOW DOES THIS WORK?

Algorithm 1 Limb darkening: compute quantitiy of photons

create photons

probability distribution for emission angle $\mu = \cos(\theta)$: $p(\mu)d\mu = \mu d\mu$

optical depth until next scattering event: $p(\tau)dt \approx e^{-\tau}d\tau$

isotropic scattering angle at low energies: $p(\mu)d\mu \approx d\mu$

follow all photons until they leave the atmosphere or are scattered back into stellar interior

10.5 Exercise 1: RNG

10.6 Exercise 2: Planck-function

- 1. analytical method
- 2. MC method

10.7 limb darkening

See section 17.

11 Introduction to Monte Carlo Radiation Transfer (Wood+)

The material is taken from

- \bullet (Wood, Wittney, Bjorkman, Wolff 2001)
- (Wood, Wittney, Bjorkman, Wolff 2013)

11.1 Elementary principles

specific intensity	$I_{ u}$
radiant energy	dE_{ν}
surface area	dA
angle	θ
solid angle	$d\Omega$
frequency range	$d\nu$
time	dt
flux	$F_{ u}$
cross section	σ
scattering angle	χ
	$\mu = \cos(\chi)$
mean intensity	J
flux	Н
radiation pressure	K

intensity	$I_{\nu}(l) = I_{\nu}(0)e^{n\sigma l}$
angular phase function of the scattering particle	$P(\cos(\chi))$

inverse method	$\xi = \int_0^{x_0} P(x)dx \text{ with } \xi \in \mathcal{U}(0,1)$
rejection method	

11.2 Eddington factors

11.3 Example: plane parallel atmosphere

- 1. emission of photons: select two angles (3D space). In isotropic scattering
 - θ met $\mu = \cos(\theta)$ - $\mu = 2\xi - 1$ (isotropic scattering) - $\mu = \sqrt{\xi}$ (A slab is heated from below. Then $P(\mu) = \mu$) • $\phi = 2\pi\xi$
- 2. propagation of photons
 - sample optical depth from $\tau = -\log(\xi)$
 - distance travelled $L = \frac{\tau z_{max}}{\tau_{max}}$

3. conclusion of emission and propagation

$$x = x + L\sin(\theta)\cos(\phi)$$

$$y = y + L\sin(\theta)\sin(\phi)$$

$$z = z + L\cos(\theta)$$
(11)

4. Binning: once the photon exists the slab. Produce histograms of the distribution function. Finally, we wish to compute the output flux or the intensity.

I have seen that a newer version of the paper is available, which was also used in these notes (which contains amongst other up-to-date references to code fragments).

A Plane Parallel, Isotropic Scattering Monte Carlo Code

11.4 Monte Carlo Radiative Transfer

From a macroscopic perspective, RT calculations rest on the transfer equation

- emissivity η (how much energy is added to radiation field due to emission)
- \bullet opacity χ (how much energy is removed due to absorption)
- the source function $S = \frac{\eta}{\chi}$
- \bullet optical depth τ captures the opaqueness of a medium

$$\left(\frac{1}{c}\frac{\partial}{\partial t} + \nabla \cdot n\right)I = \eta - \chi I \tag{12}$$

$$d\epsilon = Id\nu dt d\Omega dA.n \tag{13}$$

11.5 P Cygni profile for beta-velocity law and given opacity Monte Carlo simulation

11.5.1 Structure of the code

- module common
- module my_inter
- program pcyg
 - $-\,$ INPUT xk0, alpha, beta
 - OUTPUT
 - PROGRAM FLOW: loop over all photons
 - * get xstart and vstart

*

- then do normalisation
- function func(r)
- $\bullet \ \, function \ \, xmueout(xk0,alpha,r,v,sigma) \\$
- function rtbis(func,x1,x2,xacc)

12 Challenges in Radiative Transfer (Ivan Milic)

12.1 Overview of the problem

Forward problem

The forward problem is schematically represented

$$\xrightarrow{\vec{T}, \rho, \vec{B}, \vec{v}} \xrightarrow{\text{forward problem}} I_{\lambda}^{+} = F(\vec{T}, \rho, \vec{B}, \vec{v})$$

In fact solve for intensity vector $\vec{I} = \begin{pmatrix} I \\ Q \\ \alpha \\ V \end{pmatrix}$ obeying the equation

$$\frac{d\vec{I}}{d\tau} = -X(\vec{T}, \rho, \vec{B}, \vec{v})\vec{I} - \vec{j}(\vec{T}, \rho, \vec{B}, \vec{v})$$
 (14)

and the solution

$$I_{\lambda}^{+} = I_{0}^{+}e^{-\int} + \int \vec{j}e^{-\int}d\tau \tag{15}$$

Example Source function
$$S = a\tau + b$$
 then $\int_0^{\tau_{max}} (a\tau + b)e^{-\tau}d\tau = ...$

Inverse problem

The inverse problem is schematically represented

Via least-squares approximation

$$\min_{\vec{T},\rho,\vec{B},\vec{v}} \sum \left(I_{\lambda}^{obs} - I_{\lambda}(\vec{T},\rho,\vec{B},\vec{v}) \right)^{2} \tag{16}$$

12.2 Challenging domains of application

- Lyman alpha in Galaxy Halos
- Dusty torii (AGD)
- protoplanetary disks
- circumstellar disks
- athmospheres

September 17, 2019
13 Asymptotic Preserving Monte Carlo methods for transport equations in the diffusive limit (Dimarco+2018)

$\overset{26}{\mathbf{14}}$ Splitting methods

From notes by professor Frank.

14.1 Exercises

14.1.1 Exercise 1

Part III

Practical work and Exercises

15 Overview of exercises (PART I)

1. limb-darkening scattering exercise we did during the course. — You can look into your notes from that, and I attach here also a sample program which you can use a base. After you have familiarised yourself with this, you can start to think bout how you would go about to extend this to a 3D setting (assuming isotropic scattering).

- 2. (As prep for Monte-Carlo school) here is a script computing a UV resonance P-Cygni line in spherically symmetric wind with v beta-law. At top of routine, a few exercises are given, where you can modify and play around with code. Monte-Carlo program which computes a UV resonance spectral line from a fast outflowing spherically symmetric stellar wind (if you were not cc'd on that email, let me know so that I can send you the files as well). At the top of that little script, there are a few suggestions for exercises (additions) you could do to that program, in order to learn a bit more about the general workings of Monte-Carlo radiative transfer in this context. So that might be a good idea for you to do as well! (And you can also ask the others in the group for some tips etc. then.)
- 3. Some background reading:
 - Attached mc manual by Puls.
 - Paper by Sundqvist+ 2010 (Appendix, I think).

16 Overview of exercises (PART II)

- 1. Calculate the probability distribution to sample from in the case of Eddington limb darkening for the initial distribution (see 18.3.4).
- 2. Calculate analytical solution for simplified problem in 18.3.2 in the case that mu = 1.
- 3. Perform convergence analysis. See Section 18.3.6

17 Limb darkening

17.0.1 2D Case

We again have $\mu = \cos(\theta)$. The solution of the radiative transfer equation in <u>plane-parallel symmetry</u> with frequency-independent absorption and emission, is

$$I(\mu) = I_1(0.4 + 0.6\mu) \tag{17}$$

In the Monte Carlo code, the photons are sorted according to the direction that they leave the atmosphere.

Goal Calculates the angular dependence of photon's emitted from a plane-parallel, grey atmosphere of radial optical depth taumax. The value of tau determines the position of the photon

Variables and Algorithm

- muarray contains emergent photons
- na number of channels
- dmu = 1/na width of channels
- nphot number of photons
- taumax maximum optical depth

Algorithm 2 Limb darkening: compute quantitiy of photons

```
initialization
  radial optical depth \tau
  direction \mu
for all photons do
   \tau = \tau_{max}
    \overline{\text{while tau}} \ge 0 \text{ do}
       compute scattering angle mu
       if tau \geq taumax then |mu = sqrt(x)| (initial distribution)
       else mu = 2 * x = 1 (isotropic scattering)
       tau_i = -log(x2)
       tau = tau - tau_i*mu
   end while
   now we know that the photon has left the photosphere
   compute the distribution of all angles mu at which the photon left the photosphere
end for
visualisation:
```

- plot photon numbers from $\mu d\mu$ against mu
- plot specific intensity from $d\mu$ against mu against

Figure 1 is according to what is expected $I = I_0(0.4 + 0.6\mu)$

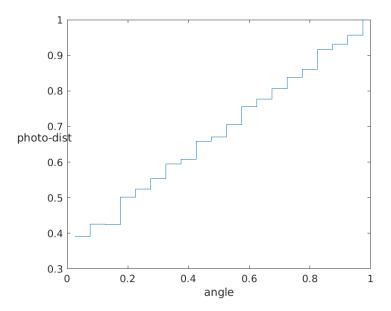


Figure 1: histogram for mu

40 35

17.0.2 3D Code

What changes is this:

- \bullet introduction of a new angle ϕ
- \bullet the optical depth has to be updated according to ϕ also

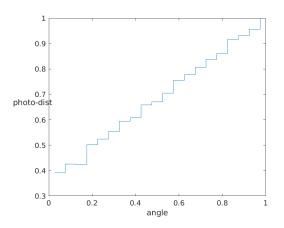


Figure 2: histogram for mu

Figure 3: histogram for phi

Figure 2 and Figure 3 are according to what is expected, namely $I=I_0(0.4+0.6\mu)$ and a uniform distribution for phi, which corresponds to a $I\sim\frac{1}{\phi}$

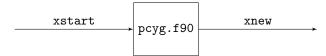
${}^{30}_{18}$ Investigation of program: pcyg.f90

18.1 Overview of variables

name	explanation
	paramaters
xk0	
alpha	velocity profile parameter
beta	velocity profile parameter
sta	rt frequency of the photon
xstart	start frequency
vmin	
vmax	
	angle of the photon
xmuestart	start angle
xmuein	incident angle
xmueou	outward angle
pstart	impact parameter
xnew	new photon frequency
	optical depth
tau	optical depth
n	umber of photons admin
nphot	number of photons
nin	photons scattered back into core
nout	photons escaped
	functions
func	velocity profile
	distance from center of star r
xmueout	outwards (scattered) angle
	xk0
	alpha
	r
	v
	sigma

18.2 Mathematical things that are noteworthy

18.2.1 General working



The photons are sorted according to xnew. In general, the flux is dependent on μ and the frequency x.

make formula

- I think that it satisfies $N(x)dx \sim I(x)xdx$
- $\bullet\,$ We are thus interested in $F_\lambda=F_\nu$

18.2.2 Practical formula

- emission angle $\mu = \cos(\theta)$
- according p-ray $p = \sqrt{1 \mu^2} = \sin(\theta)$
- incident angle xmuein = $\sqrt{1 \left(\frac{pstart}{r}\right)^2}$

18.2.3 Geometry & Symmetry assumptions

• spherical geometry

18.3 Exercises

18.3.1 Investigation of original code

In original version of the code, all photons are released isotropially from the photosphere.

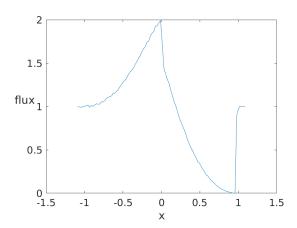
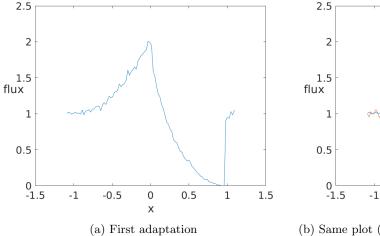


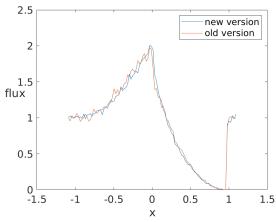
Figure 4: Original version of the code

18.3.2 First adaptation: what if all photons are released radially from photosphere?

Release photons radially: numerical MC experiments What would happen with line-profile, if you assumed all photons were released radially from photopshere?

- In other words xmuestart = 1. Results in Figure 5.
- This is implemented under the test case test_number=1.





(b) Same plot (together with output of initial version)

Figure 5: The number of photons equals 10^5

Derive analytic expression See also slide 26/49 [Sundqvist course material].

• since xmuein = 1 we have for the velocity profile

$$v = v_{\infty} (1 - b/r)^{\beta} \tag{18}$$

A scaled version of Equation (18) yields

$$u = \frac{v(r)}{v_{\infty}} = \left(1 - \frac{r_{\infty}}{r}\right)^{\beta} \tag{19}$$

with $u \in [0..1]$

- Doppler shift for the frequency of the photons: $x_{CMF} = x_{REF} \mu u$.
- Condition for resonance from Sobolov approximation (to be studied later): $x_{CMF} = 0$ thus

$$x_{REF} = \mu u \tag{20}$$

or thus $x_{REF} = \boxed{u_{\text{interaction}}}$ and than solve Equation 19 for $r_{\text{interaction}}$

• If $\mu = 1$ then

$$x = \left(1 - \frac{r_{\infty}}{r}\right)^{\beta}$$

$$x^{-\beta} = 1 - \frac{r_{\infty}}{r}$$
(21)

$$r(1-x^{-\beta}) = r_{\infty}$$

$$r(x) = \frac{r_{\infty}}{1 - x^{-\beta}} \tag{22}$$

 \bullet From the location of interaction r, the incident angle can be calculated

$$xmuein = \sqrt{1 - \left[\frac{pstart}{r}\right]^2} = \sqrt{1 - \left[\frac{\sqrt{1 - xmuestart^2}}{r}\right]^2}$$
 (23)

Now also taking into account that xmuestart = 1 then yields

$$xmuein = 1$$
 (24)

• The calculation of the optical depth goes as follows:

$$\tau = \frac{\text{xk0}}{rv^{2-\alpha}(1 + \text{xmuein}^2\sigma)} \tag{25}$$

Now also taking into account that xmuestart = 1 gives

$$\tau = \frac{\text{xk0}}{rv^2(1+\sigma)} \tag{26}$$

where
$$v(x) = \left(1 - \frac{b}{r}\right)^{\beta}$$
 and $\frac{dv}{dr} = \frac{\beta b}{r^2} \left(1 - \frac{b}{r}\right)^{\beta - 1}$ and $\sigma(x) = \frac{dv}{dr} \frac{r}{v} - 1$ thus $\sigma(x) = \frac{\beta b}{r} \left(1 - \frac{b}{r}\right)^{-1}$

- Assuming that $\beta = 1$ then $v(x) = 1 \frac{b}{r}$ and $\frac{dv}{dr} = \frac{\beta b}{r^2}$ and $\sigma(x) = \frac{\beta b}{r}$.
- Conclusion: $\tau(x)$ is only dependent on x and not on xmuestart or xmuein.
- $\bullet\,$ xmueou follows the distribution as given by the function <code>xmueout</code>, namely

$$p(x) = \frac{1 - e^{-\tau}}{\tau} \tag{27}$$

with $\tau = \frac{\tan 0}{1 + X^2 \sigma}$ where X is a random number, so actually this comes down to

$$p(x) = \frac{1 - e^{-\frac{\tau_0}{1 + x^2 \sigma(x)}}}{\frac{\tau_0}{1 + x^2 \sigma(x)}}$$
(28)

 \bullet Finally one can combine these results to get the distribution of the photons according to the frequency x via the relation

In words, we initially have an isotropic distribution for xstart. The number of photons that are leaving the atmosphere at different frequencies is however not isotropic through complex interactions that are incorporated into p(x). One must also take into account that not all of the photons that are released actually escape from the atmosphere and also that sometimes no resonance is possible, and then Equation (29) is not applicable.

TO DO: proceed from this to the analytical expression for the flux. Here I am stuck for the moment.

Via this link, you can go back to the exercises overview: Section 16.

18.3.3 Second adaptation: isotropic scattering

What would happen to line-profile, is you assumed scattering was isotropic (i.e., NOT following Sobolev-distribution)

- in the implementation, test_number = 2
- the results are shown in Figure 6.

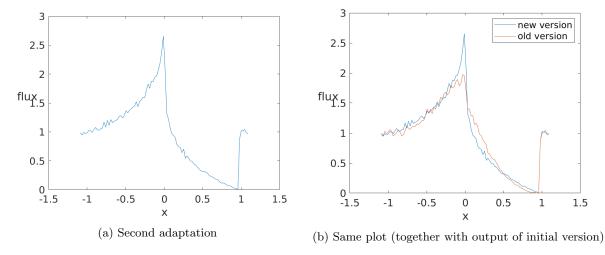


Figure 6: The number of photons equals 10^5

It is clear from Figure 6 that the peak around x = 0 is higher and sharper. Analyse this behaviour more closely

18.3.4 Third adaptation: introduction of Eddington limb-darkening

Put Eddington limb-darkening in. What happens?

General (introductory) discussion: Eddington limb darkening The data are taken from Christensen, 2015.

- the source function $S=< I>= a+b\tau_{\nu}$ with $a=\frac{\sigma}{2\pi}T_{eff}^4$ and $b=\frac{3\sigma}{4\pi}T_{eff}^4$
- solve the equation
- this yields $\frac{I(\theta)}{I(0)} = \frac{a+b\cos(\theta)}{a+b} = \frac{2}{5} + \frac{3}{5}\cos(\theta)$

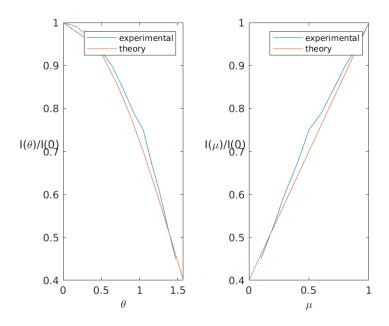


Figure 7: Eddington limb darkening (two times the same plot with $\mu = \cos(\theta)$

Construction of probability distribution corresponding to Eddington limb darkening

- 1. Let us thus first review the emmission case where the flux in each direction is isotropic i.e. $I(\theta) = I$ (as experimented in paragraph 18.3.3)
 - the specific intensity is defined as $I_{\nu}(\mu) = \frac{dE_{\nu}}{\cos(\theta)dAdtd\nu d\Omega} = \frac{dE_{\nu}}{\mu dAdtd\nu d\Omega}$
 - the flux $F_{\nu} = \int_{\Omega} I_{\nu} \cos(\theta) d\Omega$ is in this case isotropic thus

$$\xi = \int_0^\mu F_\nu d\mu = \int_0^\mu \int_\Omega I_\nu \cos(\theta) d\Omega d\mu = A \int_0^\mu \mu d\mu$$
 (30)

together with the condition that μ satisfies a probability distribution:

$$1 = \int_{-1}^{1} F_{\nu} d\mu = \int_{-1}^{1} \int_{\Omega} I_{\nu} \cos(\theta) d\Omega d\mu = \frac{A}{2}$$
 (31)

thus A=2. Photons need to be sampled according to $\mu d\mu$.

2. Now we look at a new case where the photons need to be emitted following a distribution that corresponds to $I(\theta) = I(0)(0.4 + 0.6\cos(\theta))$.

• in this case the flux $F_{\nu} = \int_{\Omega} I_{\nu} \cos(\theta) d\Omega$ is isotropic but also satisfies

$$F_{\nu} = \int_{\Omega} I_{\nu}(0)[0.4 + 0.6\cos(\theta)]\cos(\theta)d\Omega \tag{32}$$

I am not sure about the correctness of the assumption of isotropy of the flux

$$\xi = \int_0^\mu F_\nu d\mu = A \int_0^\mu (0.4 + 0.6\mu)\mu d\mu \tag{33}$$

subject to the normalisation condition -very similar to Equation (31) - that

$$1 = \int_0^1 F_{\nu} d\mu = \frac{2A}{5} \tag{34}$$

thus $A = \frac{5}{2}$. Photons need to be sampled according to

$$\frac{2}{5}(0.4 + 0.6\mu)\mu d\mu\tag{35}$$

In the code pcyg.f90 this corresponds to test_number = 3 (not yet implemented).

The results of an accept-reject method that samples the probability distribution in Equation (35).

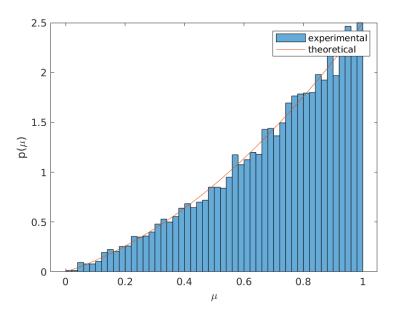


Figure 8: Accept-reject method for Eddington limb darkening

Via this link, you can go back to the exercises overview: Section 16.

18.3.5 Fourth adaptaion: photospheric line-profile

Challening: Put photospheric line-profile (simple Gaussian) in. What happens? Test on xk0=0 (opacity = 0) case.

- test case number 4
- This is still to be implemented.

18.3.6 Convergence analysis

The convergence of the Monte Carlo method is tested with the following input parameters

kx0	alpha	beta	test_number
0	0	1	0

for a varying amount of photons, as shown in Figure 9. We expect the method to have $\frac{1}{\sqrt{N}}$ convergence, where N is the number of photons. However, the methods strangely seems to have a faster convergence rate. This is still to be analysed.

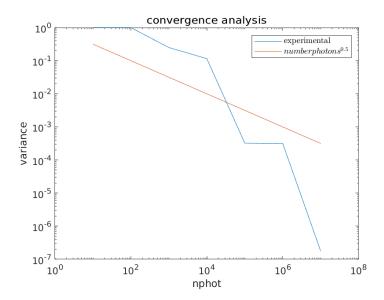


Figure 9: Original version of the code: convergence analysis (xk0=0)

Via this link, you can go back to the exercises overview: Section 16.

19 Milic Exercises

19.1 Lecture 7

- 1. Derive expressions for the emergent radiation when properties are the following:
 - ullet optically thin slab at all wavelengths
 - $\bullet \ \ {\rm wavelength\text{-}independent\ incident\ radiation}$

Solution: see slide 14?

- 2. Derive ralations between Einstein coefficients.
- 3. Calculate electron density in atmosphere from FALC model

20 Mass loss from inhomogeneous hot star winds (Sundqvist)

- GOAL: synthesis of UV resonance lines from inhomogeneous 2D winds
 - clumped in density
 - clumped in velocity
 - effects of non-void inter-clump medium
- WIND MODELS
 - symmetry assumptions
 - * 1D: spherical symmetry
 - * 2D: symmetry in Φ
 - models
 - 1. time-dependent radiation-hydrodynamic from Puls and Owocki (POF)
 - * 1D
 - * isothermal flow
 - * perturbations triggered by photospheric sound waves
 - 2. time-dependent radiation-hydrodynamic from Feldmeier (FPP)
 - * 1D
 - * treatment of energy equation
 - * perturbations triggered by photospeheric sound waves or Langevin perturbagions (photospheric turbulence)
 - 3. stochastic model, clumped in density
 - * smooth winds with $v_{\beta} = (1 b/r)^{\beta}$ with $\beta = 1$
 - * clumping factor f_{cl}
 - 4. stochastic model, clumped in density and in velocity (non-monotonic velocity field)
 - * smooth winds with $v_{\beta} = (1 b/r)^{\beta}$ with $\beta = 1$
 - * clumping factor f_{cl}
- RADIATIVE TRANSFER (MC-2D)

- ${f 21}^{42}$ Asymptotic preserving Monte Carlo methods for radiative transfer equation in diffusion limit (Dimarco+ 2018)
- 21.1 Goldstein-Taylor
- Radiative transfer 21.2

<u>September 17, 2019</u> 43

Part IV

Equation meetings

- 22 Meeting of 10 April 2019
- 23 Meeting of 17 April 2019
- 24 Meeting of 14 August 2019

Part V

Thesis meetings

25 Meeting on 6 September 2019

- $\bullet\,$ overview of Petnica summer institute on Astrophysics
- question: manual by Puls: why is isotropic distribution sampled from $\mu\mu$?
- pcyg.f90 program
- \bullet practical arangements
- SKIRT code
- $\bullet\,$ discussion of paper (Dimarco+2018)

Literature Study

- General guidelines for good practices in scientific computing are found in [Wil+14].
- I went to the 2019 Petnica Summer school in Petnica, Serbia. This was a good general introduction and overview to astrophysics.
- A very interesting article about Monte Carlo methods for radiative transfer problems, from a mathematical point of view, is [DPS18]. I am currently trying to reproduce the numerical experiments that are reported in the article.

References

- [Bus60] I. W Busbridge. The mathematics of radiative transfer. Cambridge tracts in mathematics and mathematical physics 50. Cambridge: Cambridge University press, 1960.
- [DPS18] G. Dimarco, L. Pareschi, and G. Samaey. "Asymptotic-Preserving Monte Carlo Methods for Transport Equations in the Diffusive Limit". eng. In: SIAM Journal on Scientific Computing 40.1 (2018), pp. 504–528. ISSN: 1064-8275.
- [Moe18] Nicolas Moens. Radiation-Hydrodynamics with MPI-AMRVAC: Massive-Star Atmospheres and Winds. Leuven, 2018.
- [Wik18] Wikipedia contributors. Heat flux Wikipedia, The Free Encyclopedia. [Online; accessed 14-September-2019]. 2018. URL: https://en.wikipedia.org/w/index.php?title=Heat_flux&oldid=863233807.
- [Wil+14] Greg Wilson et al. "Best Practices for Scientific Computing". In: *PLoS Biology* 12.1 (2014), pp. 1–18. ISSN: 15449173. DOI: 10.1371/journal.pbio.1001745. arXiv: arXiv: 1210.0530v4.