

Master thesis

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Exercises (part III) Via this link, you can go back to the exercises overview: see section 21.

Part I

Questions

1 Questions for professor Sundqvist

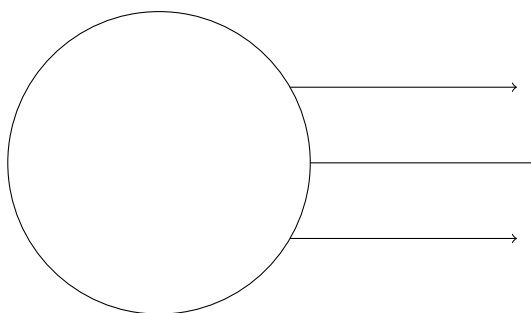
- book *Stellar Atmospheres* [Mihalas].
- What are the equations governing the processes in `pcyg.f90`

2 Questions for professor Samaey

- In [DPS18], Equation (31) why does it correspond to diffusion (more specifically the second term on the right hand side).
- 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 answer 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)
- (for which star are the experimental data and what assumptions are used in the theory?) (see ... and derive some formulas)

4 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.

$$\left[\frac{1}{c} \partial_t + \vec{n} \cdot \vec{\nabla} \right] I_\nu = \eta_\nu - \chi_\nu I_\nu \quad (1)$$

frequency	intensity	emissivity	total absorption
ν	I_ν	η_ν	χ_ν

These deliver two equations

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

$$\frac{\partial E}{\partial t} + \vec{\nabla} \cdot \vec{F} = \iint \dots d\nu d\Omega \quad (2)$$

- radiative momentum equation

$$\frac{d\vec{F}}{dt} = \iint \dots \vec{n} d\nu d\Omega \quad (3)$$

(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

$$\begin{aligned} \frac{dI}{d\tau} &= S - I \\ &= \int I d\Omega - I \end{aligned} \quad (4)$$

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.
- complex geometry difficult to show in ray-tracing scheme
- steady-state vs. time dependent
- 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 ourselves 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 $\boxed{I(\lambda, \tau_\lambda) = I_0(\lambda)e^{-\tau_\lambda} \int_0^{\tau_\lambda} S(t)e^{-t} dt}$
 - 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 Radiation equations (bis)

Material from [Iva14]

$$\frac{\delta I(q, t)}{\delta s} = \eta(q, t) - \chi(q, t)I(q, t) \quad (5)$$

In cartesian coordinates (with propagation vector $\vec{n} = \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} = \begin{bmatrix} \sin(\theta) \cos(\phi) \\ \sin(\theta) \sin(\phi) \\ \cos(\theta) \end{bmatrix}$):

$$\frac{1}{c} \frac{\partial I}{\partial t} + \sin(\theta) \cos(\phi) \frac{\partial I}{\partial x} + \sin(\theta) \sin(\phi) \frac{\partial I}{\partial y} + \cos(\theta) \frac{\partial I}{\partial z} = \eta - \chi I \quad (6)$$

- 1D planar atmosphere: $\frac{\partial I}{\partial x} = \frac{\partial I}{\partial y} = 0$:

$$\frac{1}{c} \frac{\partial I}{\partial t} + \mu \frac{\partial I}{\partial z} = \eta - \chi I \quad (7)$$

- diffusion limit

7.1.3 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	$P = \iint I_\nu n n d\nu d\Omega$
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.

$$f_\nu = \frac{K_\nu}{J_\nu} = \frac{P_\nu}{E_\nu} \quad (8)$$

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

7.1.4 Radiation transport equations, diffusion, equilibrium

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

$$\frac{dI_\nu}{ds} = j_\nu - k_\nu I_\nu \quad (9)$$

– Cartesian coordinates:

$$\boxed{\frac{\partial I_{n,\nu}}{\partial t} \frac{1}{c} + n \nabla I_{n,\nu} = j_\nu - k_{n,\nu} I_{n,\nu}} \quad (10)$$

– 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

$$\boxed{\mu \frac{dI}{dr} = j - kI} \quad (11)$$

The angle μ is constant throughout the computational domain. Dividing by k_ν , this yields

$$\mu \frac{dI}{k_\nu dr} = \mu \frac{dI}{k_\nu dz} = S - I \quad (12)$$

- 0th moment equation: integrate Equation (10) over ν and Ω , i.e. $\int d\nu d\Omega$. Conservation of energy
- first multiply Equation (10) with $\frac{n}{c}$ and then do integration

7.1.5 Radiative Diffusion Approximation

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

- on one hand, large optical depth $\tau \gg 1$: 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 $\boxed{I = B}$ or $I_\nu = B_\nu$.

$$I_\nu = B_\nu - \mu \frac{dB_\nu}{k_\nu dz} \quad (13)$$

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

7.1.6 Applications and approximations for radiative forces

- definition of general radiative acceleration vector $g = \frac{1}{\rho c} \int \int n k_\nu I_\nu d\Omega d\nu$
 - continuum Thomson scattering
 - spectral line with extinction
 - * furthermore assume central continuum source
 - * then $g_{line} = \frac{F_\nu^0 k_L}{\rho c}$
- Sobolev approximation
- CAK theory

7.1.7 Optical depth (recap)

Optical depth: physical understanding Optical depth is the ratio of incident radiant power to transmitted radiant power ([Wik19]).

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

with

- σ cross-section
- 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	
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7.3 Overview of units

opacity $\alpha = k_\nu$	$\left[\frac{m^2}{kg} \right]$
specific intensity I_ν	$\left[\frac{ergs}{cm^2.sr.Hz.s} \right] = \left[\frac{J}{cm^2.sr.Hz.s} \right]$
optical depth τ	$\boxed{\tau = 0}$ leave atmosphere

7.4 Things to know

- expanding flow: redshift (lower frequency)
- compressing flow: blueshift (higher frequency)

7.5 Definition of specific intensity

The definition of the specific intensity is

$$I_\nu = \frac{dE_\nu}{\cos(\theta) d\Omega dt d\nu} = \frac{dE_\nu}{\mu d\Omega dt d\nu} \quad (14)$$

On the other hand, for the total energy of a collection of N photons holds that

$$E_\nu = N E_{\nu, \text{photon}} \quad (15)$$

To the point From this we deduce that

$$I_\nu \mu = \frac{N(\mu) dE_{\nu, \text{photon}}}{d\Omega dt d\nu} \quad (16)$$

and thus

$$\boxed{I_{nu} \mu d\mu \sim N(\mu) d\mu} \quad (17)$$

Considering the solid angle In spherical geometry $d\Omega = \sin(\theta) d\theta d\phi = d\mu d\phi$.

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 $F_\nu = 2\pi \int_{-1}^1 I\mu d\mu = 2\pi I \frac{x^2}{2} \Big|_{-1}^1 = 0$
- 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 $P_{nu} = \frac{1}{c} \int I_0 \delta(\mu - \mu_0) n n d\Omega$
 - * 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 (11)
 - * 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 $\boxed{\frac{dE}{dr} = \frac{(j - kI)4\pi(\nu_1 - \nu_0)}{c}}$

- * 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 $\frac{dF}{dr} = \frac{(j - kI)4\pi(\nu_1 - \nu_0)n}{c}$
 - first moment equation
 - * similar reasoning
 - * $\frac{dP}{dr} = \int (j - kI) n \cdot n d\nu d\Omega$ thus $\frac{dP}{dr} = \frac{(j - kI)4\pi(\nu_1 - \nu_0)n}{c}$
 - first exercise p. 15
 - $P = \frac{1}{c} \iint I_\nu \mu^2 d\Omega d\nu = \frac{2\pi}{c} \int_{-1}^1 \int_{-1}^1 I_\nu \mu^2 d\mu d\nu = \frac{4\pi}{3c} \int B_\nu d\nu = \frac{aT^4}{3} = \frac{E}{3}$
 - 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 $\frac{1}{\kappa_R} = \frac{\int_0^\infty \frac{1}{\kappa_\nu} \frac{dB_\nu}{dT} d\nu}{\int_0^\infty \frac{dB_\nu}{dT} d\nu}$.
 - * in the diffusion limit, $F_\nu = -\frac{4\pi}{3} \frac{dB_\nu}{k_\nu dz}$ 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: $L_{SOB} = \Delta r = \frac{v_{th}}{dv/dr} = \frac{10[km/s]}{1000[km/s]/R_*} = 0.01 R_*$
 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 $\lambda_{max} T = 2897.8[\mu m K]$
 - ...
 - second exercise p.31
 - this is about the spectra of (unknown) stars
 - first exercise p.32
 - see exercise 7
 - second exercise p.32

- 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 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 $\boxed{\mu \frac{dI}{ds} = \alpha}$
 - 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 $\tau(D) \gg 1$: then $I(D) \approx S$
 - * case $\tau(D) \ll 1$: 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
- 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 23.

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
$$\mu \frac{\partial I(\tau, \mu, \phi)}{\partial \tau} = I(\tau, \mu, \phi) - \mathcal{S}(\tau, \mu, \phi)$$

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 $(1 - \omega_0 \bar{\Lambda}) \{ \text{mahtcal} S(t) \} = B(\tau)$

- * solve for $\mathcal{S}(t)$

- * 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
 - τ 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 quantity 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 23.

11 Introduction to Monte Carlo Radiation Transfer (Wood+)

The material is taken from

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

11.1 Elementary principles

specific intensity	I_ν
radiant energy	dE_ν
surface area	dA
angle	θ
solid angle	$d\Omega$
frequency range	$d\nu$
time	dt
flux	F_ν
cross section	σ
scattering angle	χ $\mu = \cos(\chi)$
mean intensity	J
flux	H
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	$\xi = \int_0^{x_0} P(x)dx$ 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

$$\begin{aligned}x &= x + L \sin(\theta) \cos(\phi) \\y &= y + L \sin(\theta) \sin(\phi) \\z &= z + L \cos(\theta)\end{aligned}\tag{18}$$

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

$$\left(\frac{1}{c} \frac{\partial}{\partial t} + \nabla \cdot \mathbf{n} \right) I = \eta - \chi I \quad (19)$$

$$d\epsilon = I d\nu dt d\Omega dA \cdot n \quad (20)$$

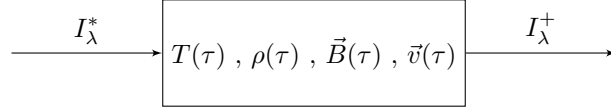
11.5 P Cygni profile for beta-velocity law and given opacity Monte Carlo simulation

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)
- function xmueout(xk0,alpha,r,v,sigma)
- function rtbis(func,x1,x2,xacc)

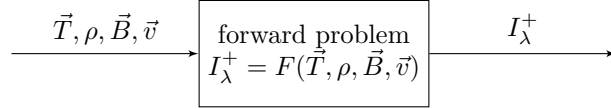
12 Challenges in Radiative Transfer (Ivan Milic)

12.1 Overview of the problem



Forward problem

The forward problem is schematically represented



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

$$\frac{d\vec{I}}{d\tau} = -X(\vec{T}, \rho, \vec{B}, \vec{v})\vec{I} - \vec{j}(\vec{T}, \rho, \vec{B}, \vec{v}) \quad (21)$$

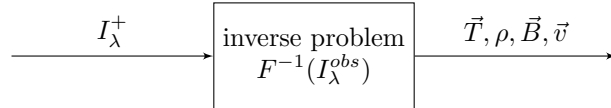
and the solution

$$I_{\lambda}^+ = I_0^+ e^{-\int} + \int \vec{j} e^{-\int} d\tau \quad (22)$$

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

Inverse problem

The inverse problem is schematically represented



Via least-squares approximation

$$\min_{\vec{T}, \rho, \vec{B}, \vec{v}} \sum \left(I_{\lambda}^{obs} - I_{\lambda}(\vec{T}, \rho, \vec{B}, \vec{v}) \right)^2 \quad (23)$$

12.2 Challenging domains of application

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

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

14 Fluid and hybrid Fluid-Kinetic models (for neutral particles in plasma edge) (Horsten2019)

The material is mainly taken from [HorstenNiels2019].

- Kinetic Boltzmann equation: neutral velocity distribution $f_n(r, v)$
- If you taken into account (e.g. microscopic processes for atomic deuterium) then the kinetic Boltzmann equation becomes

$$v \nabla f_n(r, v) = S_r(r, v) + S_{cx}(r, v) - f_n(r, v)(R_{cx}(r, v) + R_i(r)) \quad (24)$$

- Numerical solution strategies
 - finite differences/volumes/elements :computationally infeasible
 - spectral methods (series expansion of $f_n(r, v)$): not suitable for modelling discontinuities
 - stochastic approach: the whole velocity distribution is discretized by finite set of particles
- from Equation (24), the fluid model and the hybrid model is derived.
 - Fluid model: 3 state equations (continuity - momentum - energy) with boundary conditions
 - * pure-pressure equation: maximum error of 10 - 28 %
 - * with parallel momentum source: error 10 %
 - * with ion energy source: error 30 %
 - hybrid model based on micro-macro decomposition

15 Splitting methods

From notes by professor Frank.

15.1 Exercises

15.1.1 Exercise 1

16 Overview of existing (Monte Carlo) radiative transfer codes

16.1 Synthesis codes

As is pointed out in [Chr15], there are basically two methods to solve the radiative transfer problem: ray-tracing and Monte Carlo methods.

- RADICAL [**RADICAL**] (Ray-tracing, 2D, multi-purpose)
- MULTI [Car] [Car86] (computer program for solving multi-level non-LTE radiative transfer problems in moving or static atmospheres, very old: Uppsala 1986 - 1995)
- SKIRT [CB2] (continuum (Monte Carlo) radiation transfer in dusty astrophysical systems, such as spiral galaxies and accretion disks, from Ugent)
- TORUS [Har+19] (Monte Carlo radiation transfer and hydrodynamics code. Adopts 1D, 2D, 3D adaptive mesh refinement. Suitable for radiative equilibrium and creation of synthetic images and SED)
- RADMC-3D [Dul17] (Monte Carlo code that is especially applicable for dusty molecular clouds, protoplanetary disks, circumstellar envelopes, dusty tori around AGN and models of galaxies. Python interface with Fortran main code)
- TLUSTY and SYNSPEC [HL17a], [HL17b], [HL17c].

16.2 Inversion codes

- VFISV
- ASP/HAO
- HeIIX+
- SNAPI (not publicly available, created by Ivan Milic)
- multiple codes available from Instituto de Astrofísica de Canarias (IAC)
- STiC: the Stockholm inversion code

17 Integral equations

Based on the book [Mmfp].

1. integral equation from differential equation
2. types of integral equations
3. operator notation and existence of solutions
4. closed-form solutions
 - separable kernels
 - integral transform method (Fourier transform)
 - differentiation
5. Neumann series
6. Fredholm theory
7. Schmidt-Hilbert theory

Fredholm equation first kind

$$0 = f + \lambda \mathcal{K}y \tag{25}$$

Fredholm equation second kind

$$y = f + \lambda \mathcal{K}y \tag{26}$$

18 Master thesis discussions

limb darkening

- the integro-differential equation describing radiative transfer

$$\begin{aligned}\frac{dI}{d\tau} &= -I + S \\ &= -I + \frac{1}{4\pi} \int I d\Omega\end{aligned}\tag{27}$$

- The difficulty resides in the source function
- Monte Carlo simulation avoids explicit source function: source function implicit in Monte Carlo simulation
- in the Monte Carlo program, the physics are simulated IN BETWEEN TWO CONSECUTIVE SCATTERING EVENTS as follows

$$\frac{dI}{dz} = -\alpha I\tag{28}$$

thus $\frac{dI}{I} = -\alpha dz = -\delta\tau$ and $I = I_0 e^{-\delta\tau}$ and thus τ is sampled according to $\tau = -\log(X_{\text{random}})$

Part III**Practical work and Exercises****19 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 as a base. After you have familiarised yourself with this, you can start to think about 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).

20 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 Section [24.3.4](#)).
 - finished + Ok
2. Calculate analytical solution for simplified problem in the case that $\mu = 1$ (see Section [24.3.2](#)).
 - finished + Ok + can be further studied
3. Perform convergence analysis (see Section [24.3.6](#)).

21 Overview of exercises (PART III)

1. Revisit 3D limb darkening. ϕ should be sampled between 0 and 2π (see Section [23.0.2](#)). (OK)
2. Revisit convergence analysis: adapt plot formatting and standard deviation is defined as square root of variance (see Section [24.3.6](#)).
3. Test variance reduction technique (see Section [24.3.7](#)).
4. Some general considerations about the definition of specific intensity (see Section [7.5](#)). (OK)
5. For the Monte Carlo approximation of the diffusion equation, why do we have $N \sim \tau$ for low optical depth $\tau \ll 1$ (see Section [26](#)).
6. Revisit the radial streaming approximation in `pcyg.f90` for lower optical depth (e.g. `xk0=0.5`). (see Section [24.3.2](#)).
7. What happens when you add a line (e.g. $x = 0.5 = a$)? How would you do that? (see Section [25.0.1](#))
8. Towards a mathematical description of the problem.

22 Overview of exercises (PART IV)

1. Convergence analysis: also fit a line through the points (see Section 24.3.6). Formally, we write $V = CN^x$ and determine both C and X from experimental data. Correspondingly, $\log(V) = \log(C) + x \log(N)$. This is fitted using least-squares.
2. Variance reduction technique
 - averaging over different stochastic realizations?
 - take `xk0=0.5`
 - try to also discretize μ
3. Adding a second line: develop computer code in the radial streaming assumption (use analytic formulas) $\mu = 1$ (see Section 25).
 - a following improvement is the use of a grid instead of using the bisection method.

23 Limb darkening program

23.0.1 2D Case

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

$$I(\mu) = I_1(0.4 + 0.6\mu) \quad (29)$$

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 quantity of photons

```

initialization
  radial optical depth  $\tau$ 
  direction  $\mu$ 
for all photons do
   $\tau = \tau_{max}$ 
  while  $\tau \geq 0$  do
    compute scattering angle  $\mu$ 
    if  $\tau \geq \text{taumax}$  then  $\mu = \text{sqrt}(x)$  (initial distribution)
    else  $\mu = 2 * x - 1$  (isotropic scattering)
     $\tau_i = -\log(x^2)$ 
     $\tau = \tau - \tau_i * \mu$ 
  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 $I = I_0(0.4 + 0.6\mu)$. The input parameters are as follows
`LimbDarkening(number_of_channels = 20, number_of_photons = 10^5 ,
maximum_optical_depth = 10).`

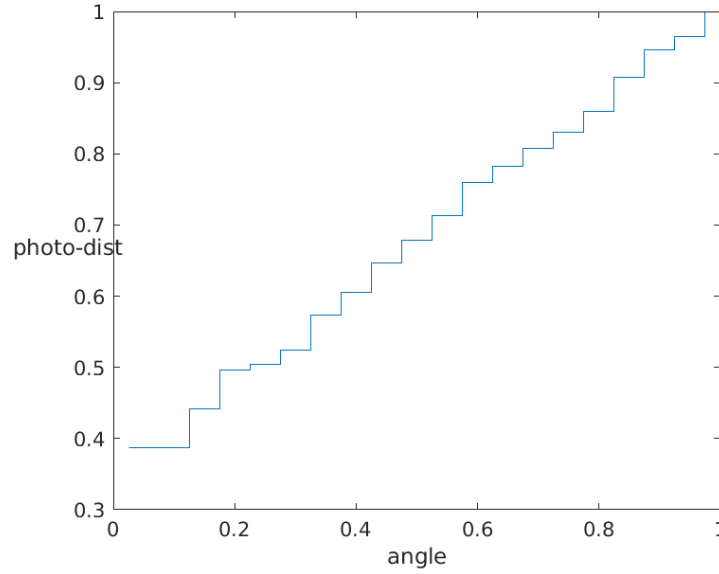


Figure 1: histogram for mu

23.0.2 3D Code

What changes is this:

- introduction of a new angle ϕ
- the optical depth is not updated with respect to ϕ

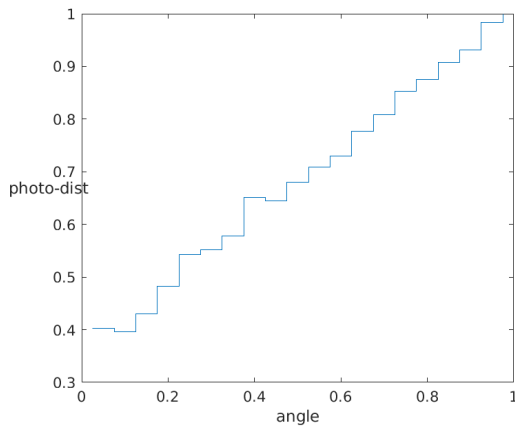


Figure 2: histogram for mu

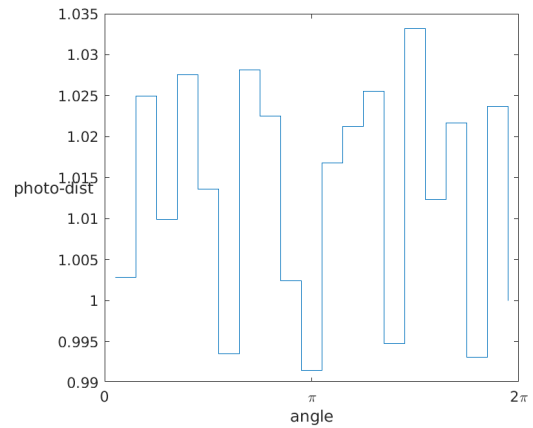


Figure 3: histogram for phi

Figure 2 and Figure 3 are the result of the function `Limb_Darkening_3D` with the following input parameters: `Limb_Darkening_3D(number_of_channels = 20, number_of_photons = 105, maximum_optical_depth = 10)`. The results according to what is expected, namely $I = I_0(0.4 + 0.6\mu)$ and ϕ follows a uniform distribution.

Extension: make version where the optical depth is updated with respect to ϕ

Via this link, you can go back to the exercises overview: [Section 21](#).

24 Spectral line formation: pcyg.f90

This section is about the study of line formation in an expanding wind.

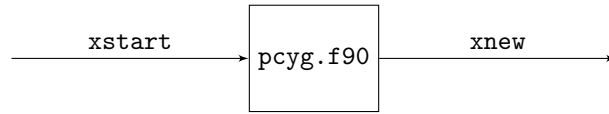
24.1 Overview of variables

name	explanation
paramaters	
xk0	
alpha	velocity profile parameter
beta	velocity profile parameter
start 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
number 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

The amout of bins `nchan` = 100.

24.2 Mathematical things that are noteworthy

24.2.1 General working



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

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

24.2.2 Practical formula

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

24.2.3 Geometry & Symmetry assumptions

- spherical geometry

24.3 Exercises

24.3.1 Investigation of original code

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

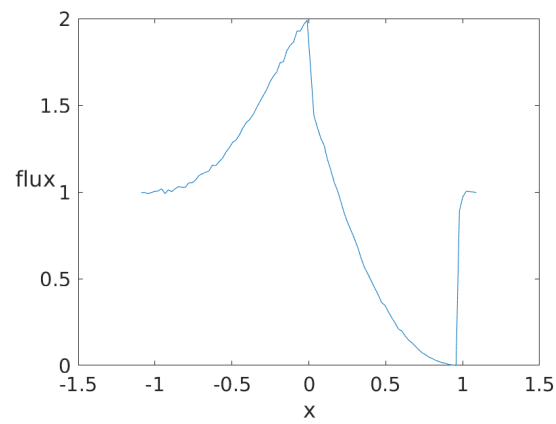


Figure 4: Original version of the code

24.3.2 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`.
- This is implemented under the test case `test.number=1`.
- Results in Figure 5 for opacity `xk0 = 100`.

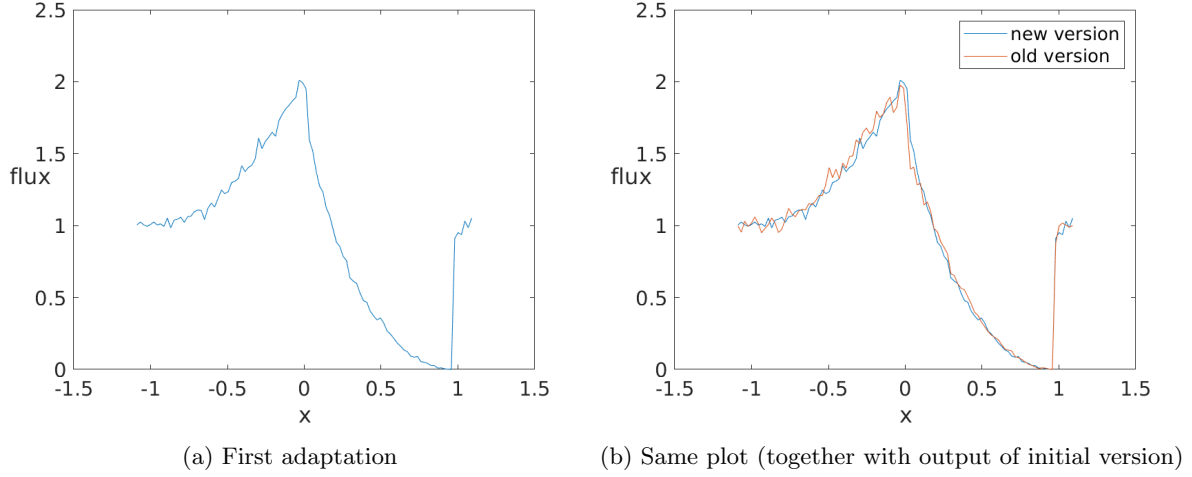


Figure 5: The number of photons equals 10^5 , `xk0=100`

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

- since `xmuein = 1` we have for the velocity profile

$$v = v_{\infty} (1 - b/r)^{\beta} \quad (30)$$

A scaled version of Equation (30) yields

$$u = \frac{v(r)}{v_{\infty}} = \left(1 - \frac{r_{\infty}}{r}\right)^{\beta} \quad (31)$$

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

$$x_{REF} = \mu u \quad (32)$$

or thus $x_{REF} = u_{\text{interaction}}$ and than solve Equation 31 for $r_{\text{interaction}}$

- If $\mu = 1$ then

$$x = \left(1 - \frac{r_{\infty}}{r}\right)^{\beta} \quad (33)$$

$$x^{1/\beta} = 1 - \frac{r_{\infty}}{r}$$

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

$$r(x) = \frac{r_{\infty}}{1 - x^{1/\beta}} \quad (34)$$

attention, here was something wrong!

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

$$\mathbf{xmuein} = \sqrt{1 - \left[\frac{\mathbf{pstart}}{r} \right]^2} = \sqrt{1 - \left[\frac{\sqrt{1 - \mathbf{xmuestart}^2}}{r} \right]^2} \quad (35)$$

Now also taking into account that $\mathbf{xmuestart} = 1$ then yields

$$\mathbf{xmuein} = 1 \quad (36)$$

- The calculation of the optical depth goes as follows:

$$\tau = \frac{\mathbf{xk0}}{rv^{2-\alpha}(1 + \mathbf{xmuein}^2\sigma)} \quad (37)$$

Now also taking into account that $\mathbf{xmuestart} = 1$ gives

$$\tau = \frac{\mathbf{xk0}}{rv^2(1 + \sigma)} \quad (38)$$

where $\boxed{v(x) = \left(1 - \frac{b}{r}\right)^\beta}$ 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 $\boxed{\sigma(x) = \frac{\beta b}{r} \left(1 - \frac{b}{r}\right)^{-1}}$

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

$$p(x) = \frac{1 - e^{-\tau}}{\tau} \quad (39)$$

with $\tau = \frac{\mathbf{tau0}}{1 + \mathbf{X}^2\sigma}$ where \mathbf{X} is a random number, so actually this comes down to

$$\boxed{p(x) = \frac{1 - e^{-\frac{\tau_0}{1+x^2\sigma(x)}}}{\frac{\tau_0}{1+x^2\sigma(x)}}} \quad (40)$$

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

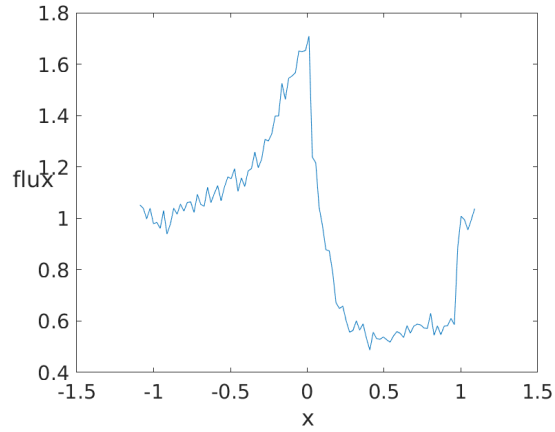
$$\mathbf{xnew} = \mathbf{xstart} + v(\mathbf{xmueou} - \mathbf{xmuein}) = \mathbf{xstart} + v(\mathbf{xmueou} - 1) \quad (41)$$

In words, we initially have an isotropic distribution for \mathbf{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 (41) is not applicable.

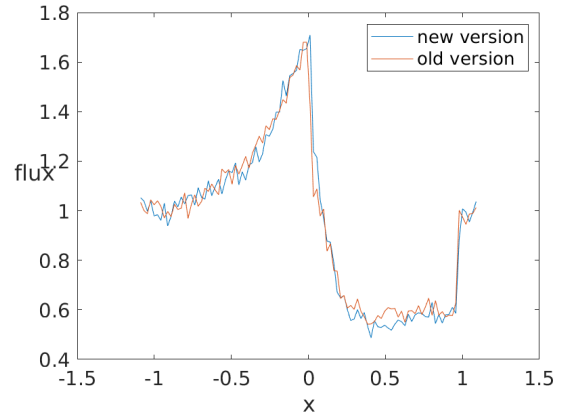
TO DO: proceed from this to the analytical expression for the flux. Here I am stuck for the moment.

Via this link, you can go back to the exercises overview: [Section 20](#).

Experiments with other opacities The results for $xk0=0.5$ are shown in Figures 6 and 7.



(a) First adaptation



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

Figure 6: The number of photons equals 10^5 , $xk0=0.5$

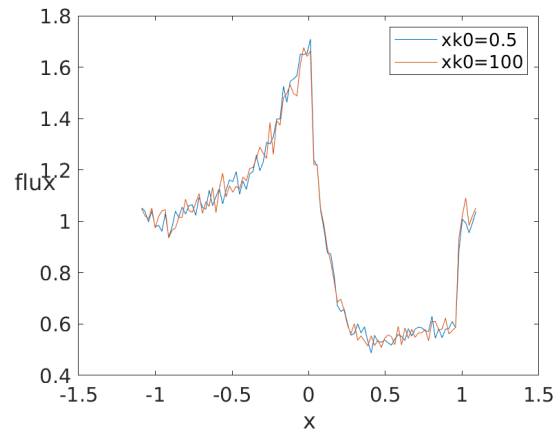


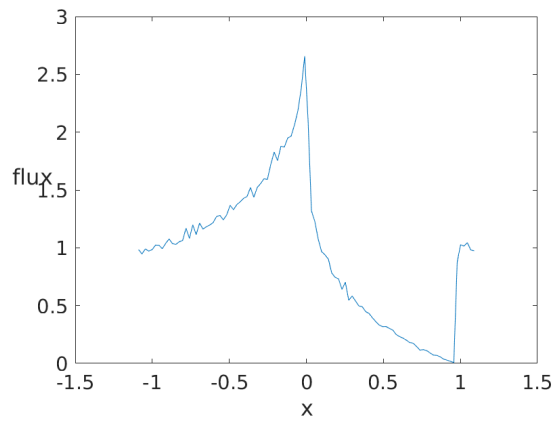
Figure 7: The number of photons equals 10^5 , $xk0=0.5$

Via this link, you can go back to the exercises overview: [Section 21](#).

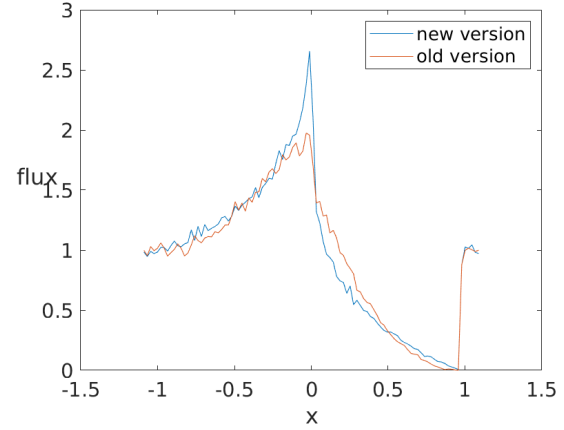
24.3.3 Second adaptation: isotropic scattering

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

- in the implementation, `test_number = 2`
- the results are shown in Figure 8.



(a) Second adaptation



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

Figure 8: The number of photons equals 10^5

It is clear from Figure 8 that the peak around $x = 0$ is higher and sharper.

Analyse this behaviour more closely

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

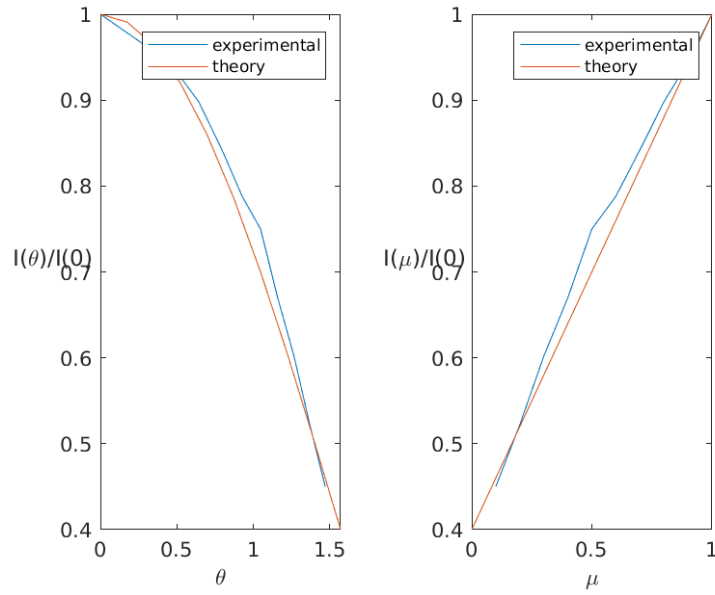


Figure 9: Eddington limb darkening (two times the same plot with $\mu = \cos(\theta)$)

Construction of probability distribution corresponding to Eddington limb darkening

1. Let us thus first review the emission case where the flux in each direction is isotropic i.e. $I(\theta) = I$ (as experimented in paragraph 24.3.3)

- 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

$$\xi = \int_0^\mu F_\nu d\mu = \int_0^\mu \int_\Omega I_\nu \cos(\theta) d\Omega d\mu = A \int_0^\mu \mu d\mu \quad (42)$$

together with the condition that μ satisfies a probability distribution:

$$1 = \int_{-1}^1 F_\nu d\mu = \int_{-1}^1 \int_\Omega I_\nu \cos(\theta) d\Omega d\mu = \frac{A}{2} \quad (43)$$

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

$$F_\nu = \int_{\Omega} I_\nu(0)[0.4 + 0.6 \cos(\theta)] \cos(\theta) d\Omega \quad (44)$$

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

$$\xi = \int_0^\mu F_\nu d\mu = A \int_0^\mu (0.4 + 0.6\mu) \mu d\mu \quad (45)$$

subject to the normalisation condition -very similar to Equation (43) - that

$$1 = \int_0^1 F_\nu d\mu = \frac{2A}{5} \quad (46)$$

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

$$\frac{2}{5}(0.4 + 0.6\mu) \mu d\mu \quad (47)$$

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 (47).

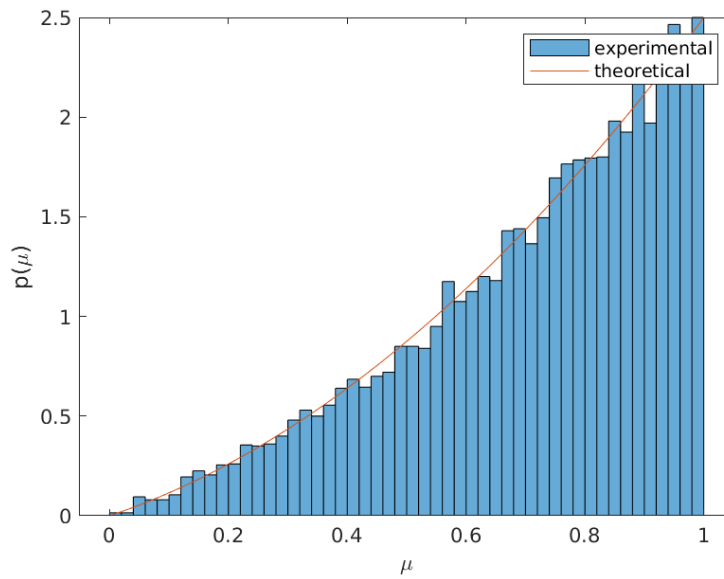


Figure 10: Accept-reject method for Eddington limb darkening

Via this link, you can go back to the exercises overview: [Section 20](#).

24.3.5 Fourth adaptaion: photospheric line-profile

Challenging: Put photospheric line-profile (simple Gaussian) in. What happens? Test on $\kappa_0=0$ (opacity = 0) case.

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

24.3.6 Convergence analysis

Zero opacity 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 11. 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.

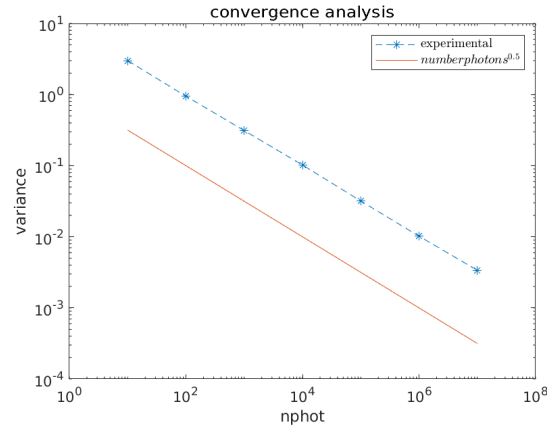


Figure 11: Original version of the code: convergence analysis (xk0=0)

Nonzero opacity The convergence test is set up as follows: different Monte Carlo simulations (with increasing number of photons) are compared to an *expensive* simulation with 10^7 photons. As can be seen in Figure 12, the spectrum profile behaves according to a $N^{0.5}$ law.

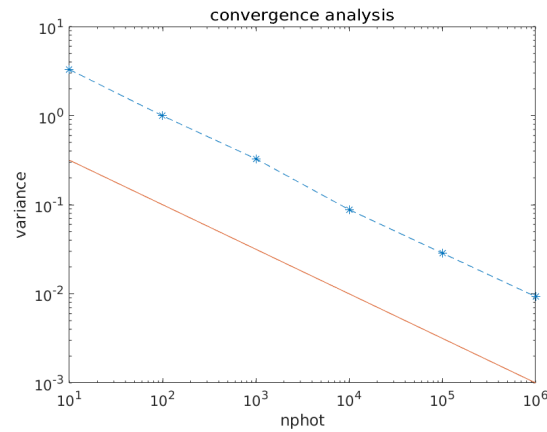


Figure 12: Original version of the code: convergence analysis (xk0=100)

Via this link, you can go back to the exercises overview: [Section 20](#).

24.3.7 Variance reduction experiment

We will set up the test as follows

- run the code with `xk0=100` and number of photons $N = 10^7$
- run the code again for lower number of photons (e.g. $N = 10^3$), both with random sampling and pseudo-random sampling
- compute variance w.r.t. *expensive* simulation and compare
- `test_number = 5`

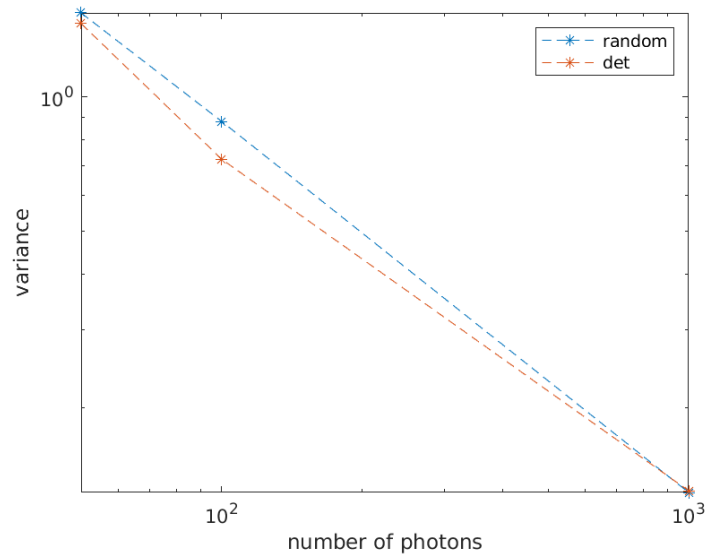


Figure 13: Original version of the code: convergence analysis (`xk0=0`)

`xk0=100`

`xk0=100`

Possible improvement: average over different stochastic realizations.

Via this [link](#), you can go back to the exercises overview: Section [21](#).

24.4 Mathematical description of the problem

Looking at literature

Have a look at [NS19].

Via this link, you can go back to the exercises overview: Section 21.

24.5 One more question

What does this mean? $x_{\text{new}} = x_{\text{start}} + (v - \text{sign}(0.06, x_{\text{mueou}})) * x_{\text{mueou}} - v * x_{\text{muein}}$

25 Dual spectral line formation

25.0.1 Introduction of second line: theoretical

What happens when you add a line (e.g. $x = 0.5 = a$)? How would you do that?

Single line

Algorithm 3 pcyg.f90: one resonance line

for all photons **do**

1. Release photon with frequency x
2. Check if interaction is überhaupt possible.
3. Solve for distance (radius r) of interaction using Sobolev approximation $x_{CMF} = x_{REL} - \mu v(r)$ with $x_{CMF} = 0$ and compute Sobolev optical depth
4. Check whether the photon is scattered:
if $\tau_S > -\log(\xi)$ **then**
 Interaction: the photon is scattered. Update the frequency
else
 No interaction
4. update the frequency according to the scattering event

end for

collect photons and perform visualisation

Introduction of second line The changes are marked in blue.

Algorithm 4 pcyg.f90: introduction of second resonance line

for all photons **do**

1. Release photon with frequency x
2. Check if interaction is überhaupt possible.
3. Solve for distance (radius r) of interaction using Sobolev approximation $x_{CMF} = x_{REL} - \mu v(r)$ with $x_{CMF} = 0$ and compute Sobolev optical depth
4. solve $x_{REF} = x_{CMF} - \mu v(r)$ with $x_{CMF} = a$ for $r_{\text{interaction}}$
5. Choose the event corresponding with the lowest value of $r_{\text{interaction}}$
6. Check whether the photon is scattered:

if $\tau_S > -\log(\xi)$ **then**

 Interaction: the photon is scattered. Update the frequency. Is there a second scattering event?

1. Check if interaction is überhaupt possible.
2. Solve $x_{REF} = x_{CMF} - \mu v(r + r_{\text{interaction}})$ with $x_{CMF} = b$ where b is the frequency where no scattering has yet found place
3. Check whether the photon is scattered:

if $\tau_{S,2} > -\log(\xi_2)$ **then**

 Second interaction: the photon is scattered once again. Update the frequency.

else

 No second interaction

else

 no interaction

end for

collect photons and perform visualisation

pitfalls yet to solve:

- root must be bracketed

Via this link, you can go back to the exercises overview: Section 21.

26 Closer look at Monte Carlo simulations

26.1 Random walk (diffusion equation)

A more simple experiment that simulates the diffusion equation (1D random walk) is also set up. The results are shown in Figure 14. We observe that $N \sim \tau^2$, as can also be derived from theory.

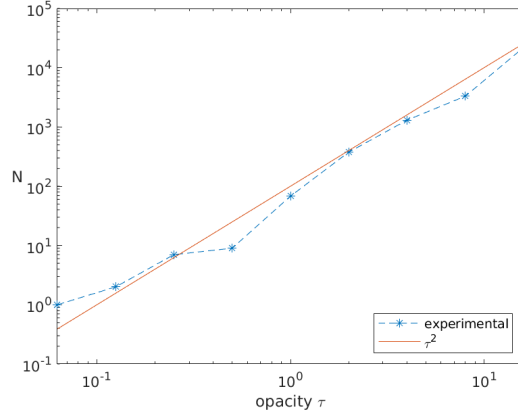


Figure 14: Number of interactions (scattering events) versus opacity, random walk

- When starting from an initial condition $x_0 = 0$ and

$$x_N = x_{N-1} \pm l \quad (48)$$

we have for the variance that $\langle x_N \rangle^2 = Nl^2$

- If we require a photon to cover a distance R then $N = \frac{R^2}{l^2}$ and

– the relation between mean-free path l and opacity α is $l = \frac{1}{\alpha}$

– with $\tau = \int_0^R \alpha ds = \frac{R}{l}$

then we have that $N = \tau^2$. This corresponds with the observations in Figure 14.

26.2 Limb darkening

We first look at results from the limb darkening program. In Figure 15, the number of scattering events is plotted versus the opacity of the medium.

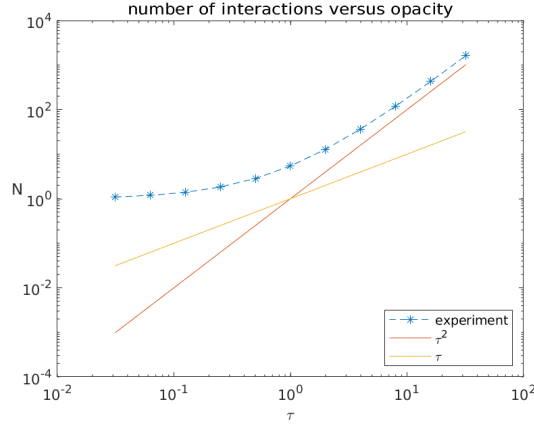


Figure 15: Number of interactions (scattering events) versus opacity, limb darkening

- For high opacity $\tau \gg 1$ we observe that $N \sim \tau$.
- However, this relationship does not hold for $\tau \ll 1$.

26.2.1 Eddington-Barbier approximation

$$J(\tau) = 3H \left(\tau + \frac{2}{3} \right) \quad (49)$$

Together with the time-independent radiative transfer equation in a gray (frequency-independent) planar medium:

$$\mu \frac{\partial I(\tau, \mu)}{\partial \tau} = I(\tau, \mu) - J(\tau, \mu) \quad (50)$$

that gives

$$\mu \frac{\partial I(\tau, \mu)}{\partial \tau} = I(\tau, \mu) - 3H \left(\frac{2}{3} + \tau \right) \quad (51)$$

with the emergent intensity $I(0, \mu)$ as solution of Equation (51). Its solution equals

$$I(\tau = 0, \mu) = I_1 \left(\frac{2}{5} + \frac{3\mu}{5} \right) \quad (52)$$

26.2.2 Validity of the Eddington-Barbier approximation

If we assume Equation (49) then $I = I_1(a + b\mu)$ thus $J = \frac{1}{2} \int (\tau, \mu) d\mu = \frac{1}{2} \int_0^1 (a + b\mu) d\mu$

26.2.3 Solving the (integro-differential) radiative transfer equation

- the integro-differential equation describing radiative transfer

$$\begin{aligned} \mu \frac{dI(\tau, \mu)}{d\tau} &= -I(\tau, \mu) + S(\tau) \\ &= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) d\Omega \end{aligned} \quad (53)$$

where $S(\tau) = \frac{1}{4\pi} \int I(\tau, \mu) d\Omega$

- The difficulty resides in the source function
- Monte Carlo simulation avoids explicit source function: source function implicit in Monte Carlo simulation
- in the Monte Carlo program, the physics are simulated IN BETWEEN TWO CONSECUTIVE SCATTERING EVENTS as follows

$$\frac{dI}{dz} = -\alpha I \quad (54)$$

thus $\frac{dI}{I} = -\alpha dz = -\delta\tau$ and $I = I_0 e^{-\delta\tau}$ and thus τ is sampled according to $\tau = -\log(X_{\text{random}})$

Analytical Solution of Equation (53) Ik heb de mosterd gehaald op [**Dublin'limb'darkening**].

$$I(0, \mu) = \int_0^\infty S(\tau) \exp\left(\frac{-\tau}{\mu}\right) d\left(\frac{\tau}{\mu}\right) \quad (55)$$

Numerical Solution of Equation (53) First rewrite the equation

$$\begin{aligned} \mu \frac{dI(\tau, \mu)}{d\tau} &= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) \sin(\theta) d\theta d\phi \\ &= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) d\mu d\phi \\ &= -I(\tau, \mu) + \frac{1}{2} \int I(\tau, \mu) d\mu \end{aligned} \quad (56)$$

Discretization scheme:

$$??? \quad (57)$$

If you assume constant opacity then $\tau = \alpha z$

27 Milic Exercises

27.1 Lecture 7

1. Derive expressions for the emergent radiation when properties are the following:

- optically thin slab at all wavelengths
- wavelength-independent incident radiation

Solution: see slide 14?

2. Derive relations between Einstein coefficients.

3. Calculate electron density in atmosphere from FALC model

28 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 photospheric sound waves or Langevin perturbations (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)

29 Asymptotic preserving Monte Carlo methods for radiative transfer equation in diffusion limit (Dimarco+ 2018)

29.1 Goldstein-Taylor

29.2 Radiative transfer

30 Do not forget

- convergence plots

Part IV

Equation meetings

- Meeting of 10 April 2019
- Meeting of 17 April 2019
- Meeting of 14 August 2019
- Meeting of 18 September 2019
- Meeting of 25 September 2019

Part V

Thesis meetings

31 Meeting on 6 September 2019

- overview of Petnica summer institute on Astrophysics
- question: manual by Puls: why is isotropic distribution sampled from $\mu\mu$?
- `pcyg.f90` program
- practical arrangements
- SKIRT code
- 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.
- [Car] Mats Carlsson. *MULTI Version 2.2*. URL: <http://folk.uio.no/matsc/mul22/mul22.html> (visited on 09/20/2019).
- [Car86] M. Carlsson. *A computer program for solving multi-level non-LTE radiative transfer problems in moving or static atmospheres*. 1986.
- [CB2] P. Camps and M. Baes. “SKIRT: An advanced dust radiative transfer code with a user-friendly architecture”. In: *Astronomy and Computing* 9 (2), pp. 20–33. ISSN: 22131337. DOI: 10.1016/j.ascom.2014.10.004. URL: <http://dx.doi.org/10.1016/j.ascom.2014.10.004>.
- [Chr15] Pinte Christophe. “Continuum radiative transfer”. eng. In: *EPJ Web of Conferences* 102 (2015), p. 00006. ISSN: 2100-014X.
- [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.
- [Dul17] Cornelis Dullemond. *RADMC-3D*. 2017. URL: <http://www.ita.uni-heidelberg.de/~dullemond/software/radmc-3d/> (visited on 09/20/2019).
- [Har+19] Tim Harries et al. “The TORUS radiation transfer code”. In: (Mar. 2019). arXiv: 1903.06672. URL: <http://arxiv.org/abs/1903.06672>.
- [HL17a] Ivan Hubeny and Thierry Lanz. “A brief introductory guide to TLUSTY and SYNSPEC”. In: (2017), pp. 1–50. arXiv: 1706.01859. URL: <http://arxiv.org/abs/1706.01859>.
- [HL17b] Ivan Hubeny and Thierry Lanz. “TLUSTY User’s Guide II: Reference Manual”. In: (2017). arXiv: 1706.01935. URL: <http://arxiv.org/abs/1706.01935>.
- [HL17c] Ivan Hubeny and Thierry Lanz. “TLUSTY User’s Guide III: Operational Manual”. In: (2017). arXiv: 1706.01937. URL: <http://arxiv.org/abs/1706.01937>.
- [Iva14] Dimitri Mihalas Ivan Hubeny. *Theory of stellar atmospheres : an introduction to astrophysical non-equilibrium quantitative spectroscopic analysis*. 2014.
- [Moe18] Nicolas Moens. *Radiation-Hydrodynamics with MPI-AMRVAC: Massive-Star Atmospheres and Winds*. Leuven, 2018.
- [NS19] Ulrich M. Noebauer and Stuart A. Sim. “Monte Carlo Radiative Transfer”. In: 5.1 (2019).
- [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.
- [Wik19] Wikipedia contributors. *Optical depth — Wikipedia, The Free Encyclopedia*. [Online; accessed 14-September-2019]. 2019. URL: https://en.wikipedia.org/w/index.php?title=Optical_depth&oldid=884427147.
- [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.