

Master thesis

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Exercises (part III) Via this link, you can go back to the exercises overview: see section [13](#).

Goal of the thesis Compute multiline transfer. With Monte Carlo techniques.

Part I

Radiative Transfer: theory

1 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.

1.1 Definition of specific intensity

The definition of the specific intensity is

$$I_\nu = \frac{dE_\nu}{\cos(\theta)d\Omega dt d\nu} = \frac{dE_\nu}{\mu d\Omega dt d\nu} \quad (1)$$

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

$$E_\nu = N E_{\nu, \text{photon}} \quad (2)$$

To the point From this we deduce that

$$I_\nu \mu = \frac{N(\mu) dE_{\nu, \text{photon}}}{d\Omega dt d\nu} \quad (3)$$

and thus

$$\boxed{I_{\nu\mu} d\mu \sim N(\mu) d\mu} \quad (4)$$

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

1.2 Radiation equations

Material from [Iva14] Specific intensity $I(s, \lambda, x, y, t)$ satisfies the Radiative Transfer Equation:

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

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
- Definition of J in Equation (3.15)

Plane parallel geometry

- 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.

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

1.3 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 $I_\nu = B_\nu$.

$$I_\nu = B_\nu - \mu \frac{dB_\nu}{k_\nu dz} \quad (9)$$

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

1.4 Applications and approximations for radiative forces

- definition of general radiative acceleration vector $g_{\text{rad}} = \frac{1}{\rho c} \int \int n k_\nu I_\nu d\Omega d\nu$

1.5 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].

1.6 Overview of symmetry assumptions

plane-parallel	1D atmosphere bounded by horizontal surfaces	
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1.7 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

1.7.1 Things to know

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

2 The mathematics of Radiative Transfer

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

2.1 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 $(1 - \omega_0 \bar{\Lambda}) \{ \mathcal{M} S(t) \} = B(\tau)$

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

- * then find $I(\tau, \mu)$

2.2 Integral equations

Based on the book [BHR02].

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

$$0 = f + \lambda \mathcal{K}y \tag{10}$$

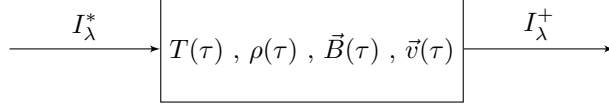
Fredholm equation second kind

$$y = f + \lambda \mathcal{K}y \tag{11}$$

3 Challenges in Radiative Transfer

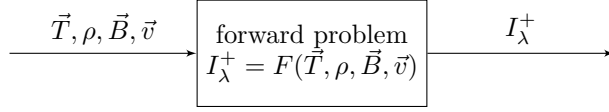
The material here originates from an oral discussion with Ivan Milic.

3.1 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

$$\frac{d\vec{I}}{d\tau} = -X(\vec{T}, \rho, \vec{B}, \vec{v})\vec{I} - \vec{j}(\vec{T}, \rho, \vec{B}, \vec{v}) \quad (12)$$

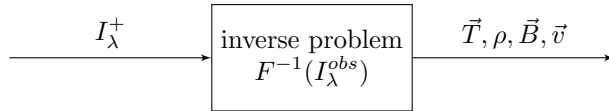
and the solution

$$I_{\lambda}^+ = I_0^+ e^{-\int} + \int \vec{j} e^{-\int} d\tau \quad (13)$$

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

$$\min_{\vec{T}, \rho, \vec{B}, \vec{v}} \sum \left(I_{\lambda}^{obs} - I_{\lambda}(\vec{T}, \rho, \vec{B}, \vec{v}) \right)^2 \quad (14)$$

3.2 Challenging domains of application

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

4 Stellar Winds

From [introStellarWindsLamersCassinelli1999]

4.1 Chronology of stellar wind studies

1. early history: similarities between spectra of nova and luminous stars
2. diagnostics of structure of outer atmospheres of the sun and stars
3. the development of the solar wind theory, further evidence for outflows
4. rocket and early satellite observations of stellar winds
5. instabilities and non-spherical effects in winds

There are still many things of stellar winds that are uncertain.

4.2 Observations & Formation of spectral lines in stellar winds

- line scattering
 - resonance scattering: from ground state of atom

4.2.1 Pcygni profiles

5 Glossary

- LASER: Light Amplification by Stimulated Emission of Radiation
- (spectral) Line-force: force on material in stellar atmosphere
- MASER: Microwave Amplification by Stimulated Emission of Radiation
- SED: spectral energy distribution

Part II

Radiative Transfer: numerical techniques

forewarned is forearmed General guidelines for good practices in scientific computing are found in [Wil+14].

6 Introduction to Monte Carlo Radiation Transfer

The material is taken from [WWBW2001] and from [WWBW2013].

6.1 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

6.2 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

$$\begin{aligned}
 x &= x + L \sin(\theta) \cos(\phi) \\
 y &= y + L \sin(\theta) \sin(\phi) \\
 z &= z + L \cos(\theta)
 \end{aligned} \tag{15}$$

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.

7 Asymptotic Preserving Monte Carlo methods for transport equations in the diffusive limit

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.

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

The material is mainly taken from [Hor19].

- 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

$$v \nabla f_n(r, v) = S_r(r, v) + S_{cx}(r, v) - f_n(r, v)(R_{cx}(r, v) + R_i(r)) \quad (16)$$

- 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 (16), 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

9 Overview of existing (Monte Carlo) radiative transfer codes

9.1 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].

9.2 Inversion codes

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

Part III**Practical work and Exercises****10 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).

11 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 [16.3](#)).
 - finished + Ok
2. Calculate analytical solution for simplified problem in the case that $\mu = 1$ (see Section [16.1](#)).
 - finished + Ok + can be further studied
3. Perform convergence analysis (see Section [16.5](#)).

12 Overview of exercises (PART III)

1. Revisit 3D limb darkening. ϕ should be sampled between 0 and 2π (see Section [15.5](#)). (OK)
2. Revisit convergence analysis: adapt plot formatting and standard deviation is defined as square root of variance (see Section [16.5](#)).
3. Test variance reduction technique (see Section [16.6](#)).
4. Some general considerations about the definition of specific intensity (see Section [1.1](#)). (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 [18](#)).
6. Revisit the radial streaming approximation in `pcyg.f90` for lower optical depth (e.g. `xx0=0.5`). (see Section [16.1](#)).
7. What happens when you add a line (e.g. $x = 0.5 = a$)? How would you do that? (see Section [17.1](#))
8. Towards a mathematical description of the problem.

13 Overview of exercises (PART IV)

1. Convergence analysis: also fit a line through the points. 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 (see Section [16.5](#)).
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 [17](#)).
 - a following improvement is the use of a grid instead of using the bisection method.
4. Limb darkening. Have a look at section 15.3.1.

14 Introductory exercises

14.1 Analytical exercises

From course material from (prof. Sundqvist - CMPAA course).

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:

- $F_x = \int_0^\pi \left[I_\nu(\theta) \sin^2(\theta) \int_0^{2\pi} \cos(\phi) d\phi \right] d\theta = 0$
- 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 $F_\nu = 2\pi \int_{-1}^1 I \mu d\mu = 2\pi I \left. \frac{\mu^2}{2} \right|_{-1}^1 = 0$

- 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 $P_{nu} = \frac{1}{c} \int I_0 \delta(\mu - \mu_0) n n d\Omega$

- * 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 (??)

- * 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

14.2 Numerical exercises

14.2.1 Implicit 1D solver

Exercise from (20-11-2018).

Goal Implement implicit solver for time-dependent diffusion equation

$$\partial_t u = \partial_{xx} u \tag{17}$$

Solution The convergence behaviour of the method is shown in Figure 1.

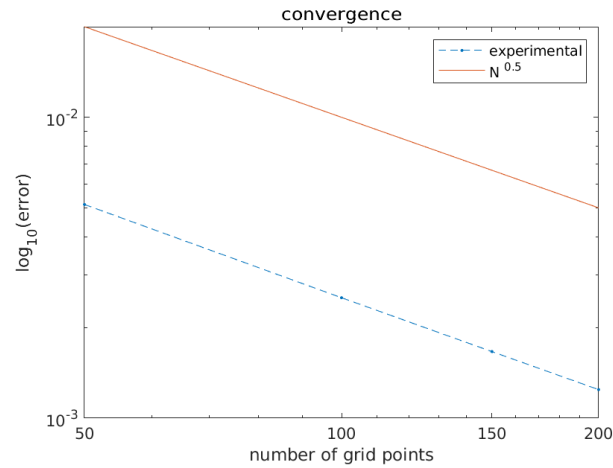


Figure 1: Convergence behaviour for 1D implicit solver (diffusion equation)

14.2.2 ADI 2D Solver

Goal Implement implicit solver for time-dependent diffusion equation

$$\partial_t u(t, x, y) = \partial_{xx} u(t, x, y) + \partial_{yy} u(t, x, y) \quad (18)$$

Solution There is still an error in the code.

14.2.3 Area of a circle

Goal Develop Monte Carlo code

Solution

14.3 Other Exercises

From course material from Ivan Milic.

14.3.1 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

15 Limb darkening

15.1 Formulation of the problem

- The radiative transfer equation 5 in this situation becomes an integro-differential equation with $S(\tau) = \frac{1}{4\pi} \int I(\tau, \mu) d\Omega$

$$\begin{aligned} \mu \frac{dI(\tau, \mu)}{d\tau} &= -I(\tau, \mu) + S(\tau) \\ &= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) d\Omega \end{aligned} \quad (19)$$

- The difficulty resides in the (evaluation of) the source function. Monte Carlo simulation avoids explicit calculation source function: source function implicit in Monte Carlo simulation. There the physics are simulated IN BETWEEN TWO CONSECUTIVE SCATTERING EVENTS as follows

$$\frac{dI}{dz} = -\alpha I \quad (20)$$

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

15.2 Solving the (integro-differential) radiative transfer equation

Analytical Solution of Equation (19) Ik heb de mosterd gehaald op [Esp].

$$I(0, \mu) = \int_0^\infty S(\tau) \exp\left(\frac{-\tau}{\mu}\right) d\left(\frac{\tau}{\mu}\right) \quad (21)$$

Numerical Solution of Equation (19) First rewrite the equation

$$\begin{aligned} \mu \frac{dI(\tau, \mu)}{d\tau} &= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) \sin(\theta) d\theta d\phi \\ &= -I(\tau, \mu) + \frac{1}{4\pi} \int I(\tau, \mu) d\mu d\phi \\ &= -I(\tau, \mu) + \frac{1}{2} \int I(\tau, \mu) d\mu \end{aligned} \quad (22)$$

Discretization scheme:

$$??? \quad (23)$$

15.3 Eddington-Barbier approximation

$$J(\tau) = 3H \left(\tau + \frac{2}{3} \right) \quad (24)$$

Together with the time-independent radiative transfer equation (5) in a gray (frequency-independent) planar medium gives

$$\mu \frac{\partial I(\tau, \mu)}{\partial \tau} = I(\tau, \mu) - 3H \left(\frac{2}{3} + \tau \right) \quad (25)$$

The emergent intensity $I(0, \mu)$ is a solution of Equation (25). Its solution for $\tau = 0$ equals

$$I(\tau = 0, \mu) = I_1 \left(\frac{2}{5} + \frac{3\mu}{5} \right) \quad (26)$$

with $a = \frac{\sigma}{2\pi} T_{eff}^4$ and $b = \frac{3\sigma}{4\pi} T_{eff}^4$

15.3.1 Validity of the Eddington-Barbier approximation

If we assume Equation (24) then $I = I_1(a + b\mu)$ thus $J = \frac{1}{2} \int (\tau, \mu) d\mu = \frac{1}{2} \int_0^1 (a + b\mu) d\mu$

dat ziet er hier niet goed uit

15.4 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

$$I(\mu) = I_1(0.4 + 0.6\mu) \quad (27)$$

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 1 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  $\mu = \sqrt{x}$  (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 2 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 = 105, maximum_optical_depth = 10)`.

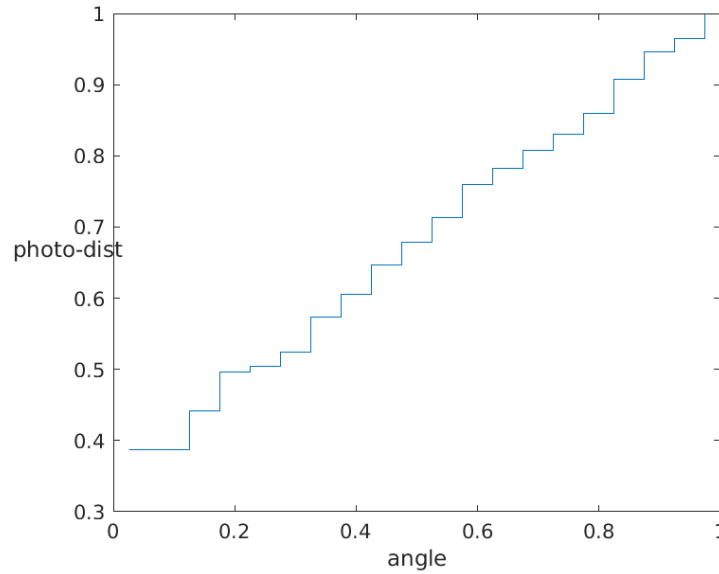


Figure 2: histogram for mu

15.5 3D Case

What changes is this:

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

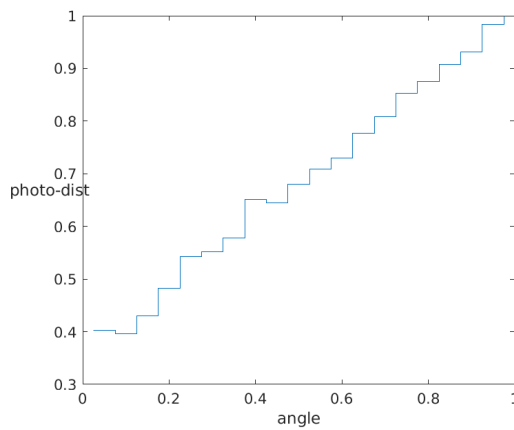


Figure 3: histogram for mu

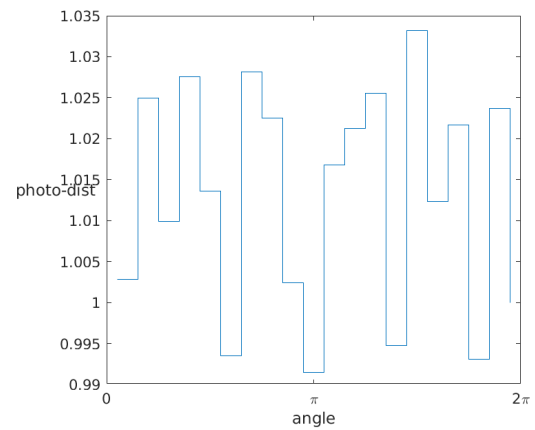


Figure 4: histogram for phi

Figure 3 and Figure 4 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 12](#).

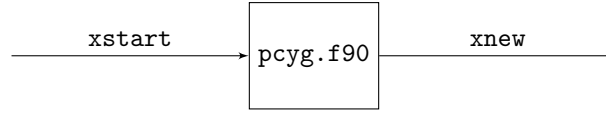
16 Spectral line formation: pcyg.f90

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

Background

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
nchan	amount of bins



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

Practical formula

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

Geometry & Symmetry assumptions

- spherical geometry

16.0.1 Experimental results

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

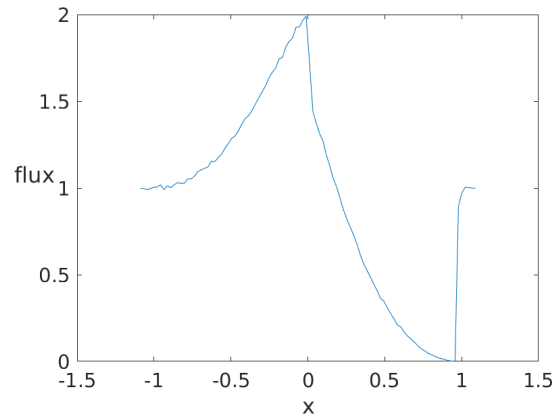


Figure 5: Original version of the code
AMOUNT OF PHOTONS?

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

16.1.1 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 6 for opacity `xk0 = 100`.

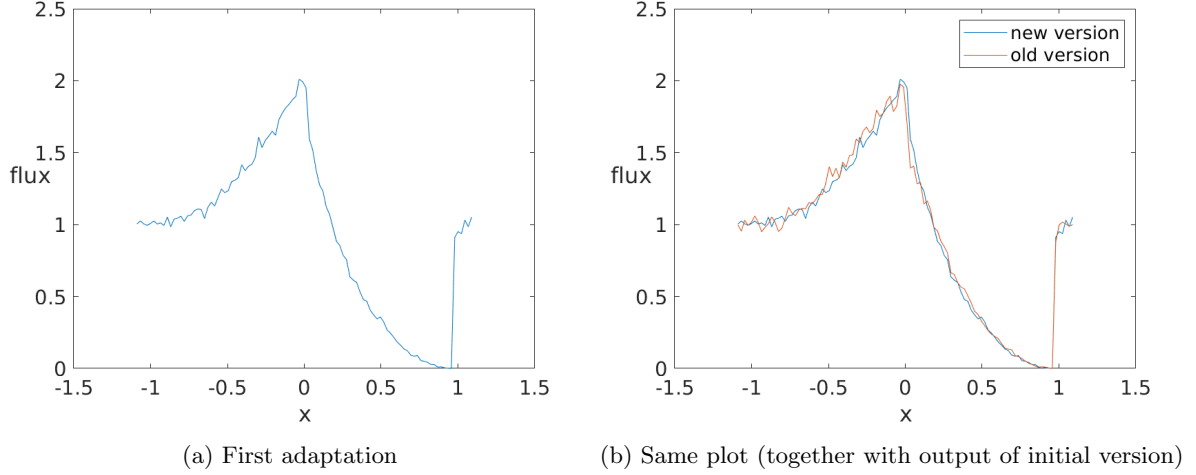


Figure 6: The number of photons equals 10^5 , `xk0=100`

16.1.2 Derive analytic expression

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

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

$$v = v_{\infty} \left(1 - b/r\right)^{\beta} \quad (28)$$

A scaled version of Equation (28) yields

$$u = \frac{v(r)}{v_{\infty}} = \left(1 - \frac{r_{\infty}}{r}\right)^{\beta} \quad (29)$$

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

$$x_{REF} = \mu u \quad (30)$$

or thus $x_{REF} = u_{\text{interaction}}$ and than solve Equation 29 for $r_{\text{interaction}}$

- If $\mu = 1$ then

$$\begin{aligned} x &= \left(1 - \frac{r_{\infty}}{r}\right)^{\beta} \\ x^{1/\beta} &= 1 - \frac{r_{\infty}}{r} \end{aligned} \quad (31)$$

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

$$r(x) = \frac{r_\infty}{1 - x^{1/\beta}} \quad (32)$$

attention, here was something wrong!

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

$$\text{xmuein} = \sqrt{1 - \left[\frac{\text{pstart}}{r}\right]^2} = \sqrt{1 - \left[\frac{\sqrt{1 - \text{xmuestart}^2}}{r}\right]^2} \quad (33)$$

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

$$\text{xmuein} = 1 \quad (34)$$

- The calculation of the optical depth goes as follows:

$$\tau = \frac{\text{xk0}}{rv^{2-\alpha}(1 + \text{xmuein}^2\sigma)} \quad (35)$$

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

$$\tau = \frac{\text{xk0}}{rv^2(1 + \sigma)} \quad (36)$$

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 .

- xmueou follows the distribution as given by the function xmueout , namely

$$p(x) = \frac{1 - e^{-\tau}}{\tau} \quad (37)$$

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

$$p(x) = \frac{1 - e^{-\frac{\tau_0}{1 + x^2\sigma(x)}}}{\frac{\tau_0}{1 + x^2\sigma(x)}} \quad (38)$$

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

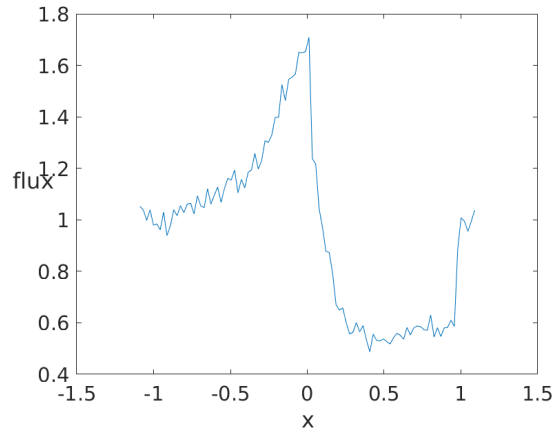
$$\text{xnew} = \text{xstart} + v(\text{xmueou} - \text{xmuein}) = \text{xstart} + v(\text{xmueou} - 1) \quad (39)$$

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 (39) is not applicable.

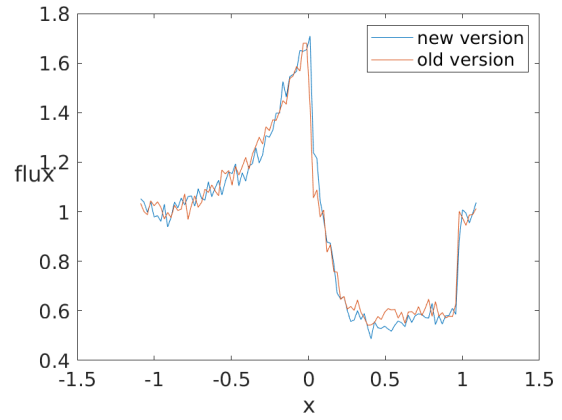
TO DO: proceed from this to the analytical expression for the flux. Here I am stuck for the moment.

16.1.3 Experiments with other opacities

The results for $xk0=0.5$ are shown in Figures 7 and 8.



(a) First adaptation



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

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

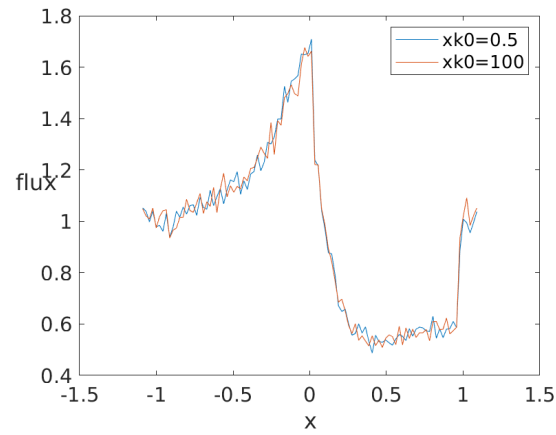


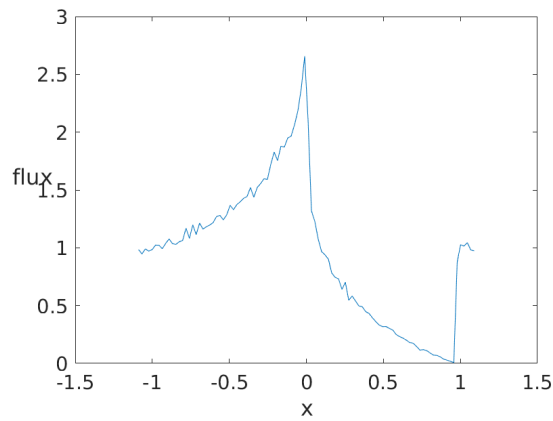
Figure 8: The number of photons equals 10^5 , $xk0=0.5$

Via this link, you can go back to the exercises overview: [Section 12](#).

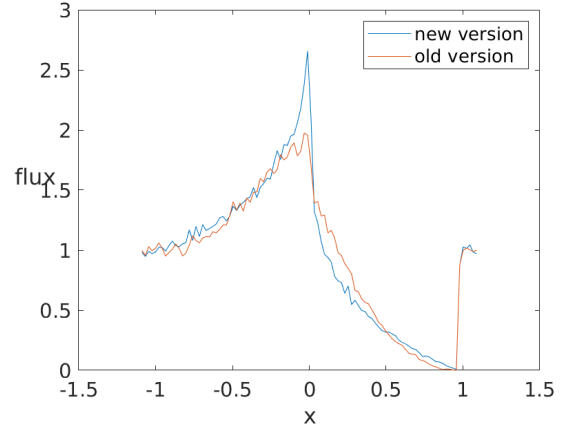
16.2 Second adaptation: isotropic scattering

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 9.



(a) Second adaptation



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

Figure 9: The number of photons equals 10^5

It is clear from Figure 9 that the peak around $x = 0$ is higher and sharper.

Analyse this behaviour more closely

16.3 Third adaptation: introduction of Eddington limb-darkening

Goal Put Eddington limb-darkening in. What happens?

16.3.1 Construction of probability distribution corresponding to Eddington limb darkening

For a general (introductory) discussion about Eddington limb darkening, please refer to Section ??

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 16.2)

- 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

$$\xi = \int_0^\mu F_\nu d\mu = \int_0^\mu \int_\Omega I_\nu \cos(\theta) d\Omega d\mu = A \int_0^\mu \mu d\mu \quad (40)$$

together with the condition that μ satisfies a probability distribution:

$$1 = \int_{-1}^1 F_\nu d\mu = \int_{-1}^1 \int_\Omega I_\nu \cos(\theta) d\Omega d\mu = \frac{A}{2} \quad (41)$$

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

$$F_\nu = \int_\Omega I_\nu(0)[0.4 + 0.6 \cos(\theta)] \cos(\theta) d\Omega \quad (42)$$

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

$$\xi = \int_0^\mu F_\nu d\mu = A \int_0^\mu (0.4 + 0.6\mu) \mu d\mu \quad (43)$$

subject to the normalisation condition -very similar to Equation (41) - that

$$1 = \int_0^1 F_\nu d\mu = \frac{2A}{5} \quad (44)$$

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

$$\frac{5}{2}(0.4 + 0.6\mu) \mu d\mu \quad (45)$$

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 (45).

Via this link, you can go back to the exercises overview: Section [11](#).

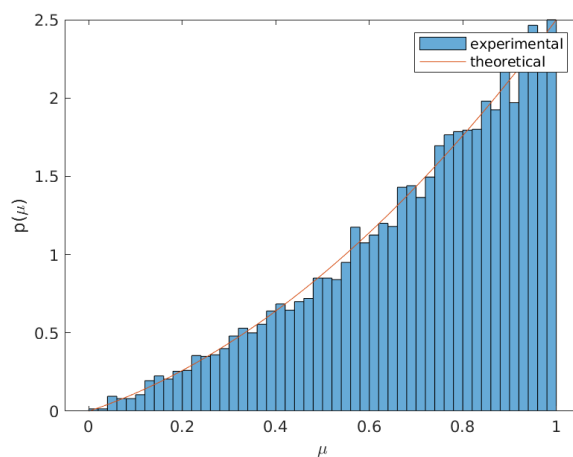


Figure 10: Accept-reject method for Eddington limb darkening

16.4 Fourth adaptaion: photospheric line-profile

Challenging: Put photospheric line-profile (simple Gaussian) in. What happens? Test on $x_{k0}=0$ (opacity = 0) case.

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

16.5 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.

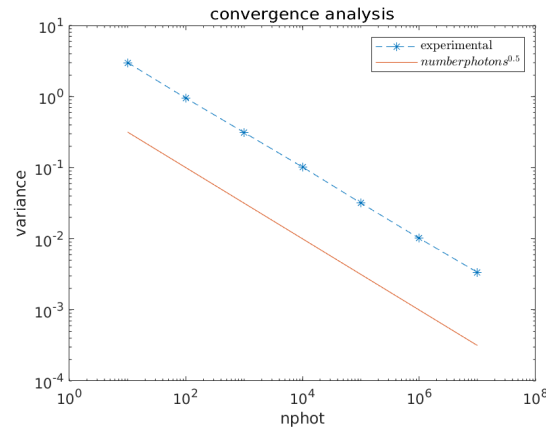


Figure 11: Original version of the code: convergence analysis (xk0=0)

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.

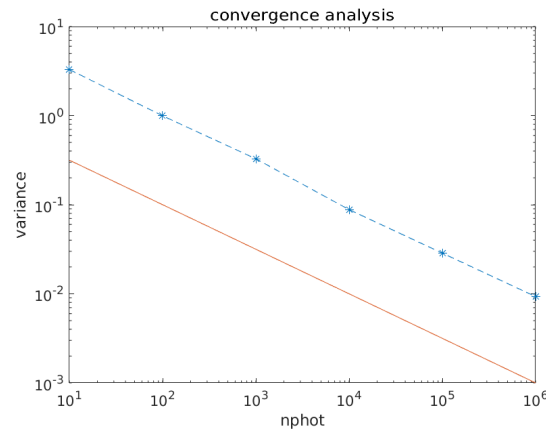


Figure 12: Original version of the code: convergence analysis (xk0=100)

Via this link, you can go back to the exercises overview: [Section 11](#).

16.6 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`

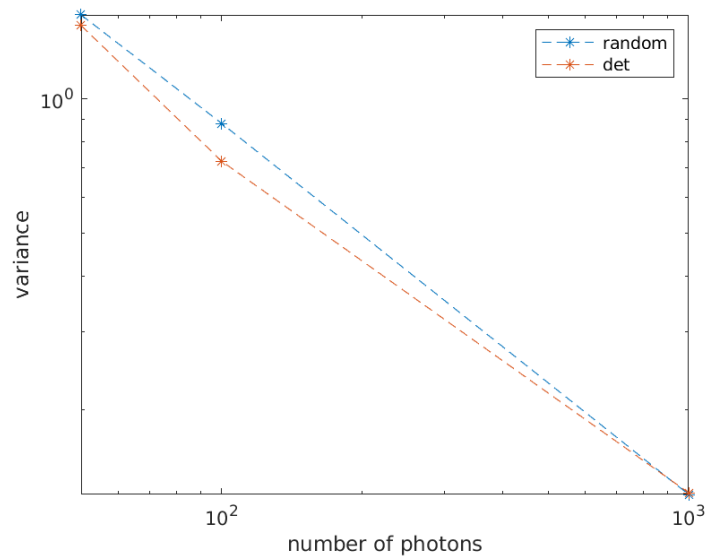


Figure 13: Original version of the code: convergence analysis (`xk0=0`)

`xk0=100` Possible improvement: average over different stochastic realizations.

Via this link, you can go back to the exercises overview: Section [12](#).

16.7 Mathematical description of the problem & Looking at literature

Have a look at [NS19] (see Appendix).

17 Dual spectral line formation

17.1 Introduction of second line: theoretical

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

17.1.1 Single line

Algorithm 2 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

17.1.2 Introduction of second line

Needs to be updated

17.2 Development of computer code

17.2.1 Implementation in Matlab: user's manual

Run the function `test_function(test_number)`.

test_number	parameter settings
0	original version
1	first adaptation: radial release
2	isotropic scattering – higher peak
3	Eddington limb darkening
4	photospheric line-profile
5	simple well
6	other resonance frequency (thus introducing shift)
7	formation of two lines, only radially streaming photons (thus also radial release)
8	formation of two lines, with radial release
9	formation of two lines, full scattering possibilities

Via this link, you can go back to the exercises overview: [Section 13](#).

17.2.2 Keeping track of the photon path

$$\begin{bmatrix} \text{xstart} \\ \text{xmuestart} \\ \text{r_new} \\ \dots \\ \text{xmueou} \end{bmatrix} \quad (46)$$

17.2.3 Dirty tricks

- when `xnew > xmax` then set `xnew` to `xmax`.

18 Closer look at Monte Carlo simulations

18.1 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.

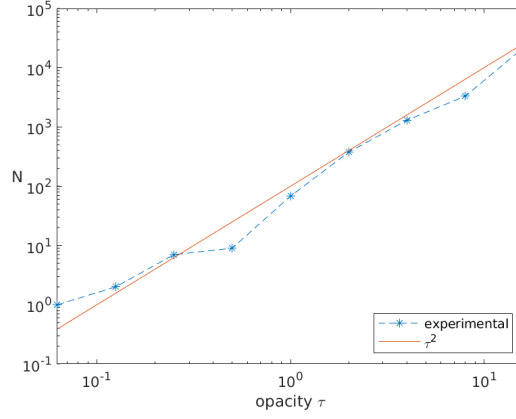


Figure 14: Number of interactions (scattering events) versus opacity, random walk

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

$$x_N = x_{N-1} \pm l \quad (47)$$

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.

18.2 Iets

18.3 Limb darkening

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

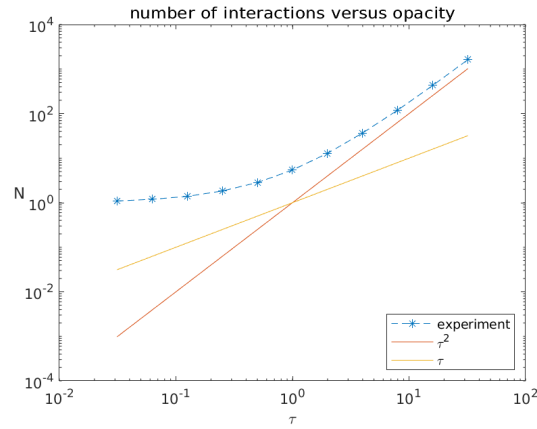


Figure 15: Number of interactions (scattering events) versus opacity, limb darkening

- For high opacity $\tau \gg 1$ we observe that $N \sim \tau$.
- Bridging regime.
- For opacity $\tau \ll 1$ we observe that $N \sim 1$: namely the photons travels very far during the first emission event.

The splitting scheme from [DPS18] can perfectly be applied to the used Monte Carlo code.

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

Part IV

Questions

19 Questions for professor Sundqvist

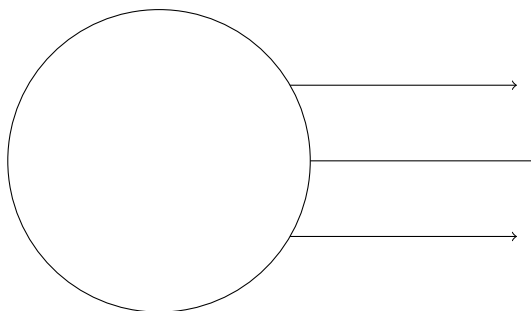
- What are the equations governing the processes in `pcyg.f90`
- What does this mean? `xnew=xstart+(v-sign(0.06,xmueou))*xmueou-v*xmuein`
- Pcygni profiles: Why don't we just take the absorption and the emission and add them together.

20 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?

21 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)
- book *Stellar Atmospheres* [Mihalas] (bought)
- ordering of array `freq` (adapted the code, experimented with it)
 - why `freq(1) = xmax-5*deltax`?
 - frequency binning: how are you sure that no lower/higher frequencies can occur?

derive this analytically
- Pcyg.f90 does it take into account that photons are scattered away from the observer? (via assumption of radial symmetry)

22 Interesting problems

- inverse radiative transfer problem

might be interesting for looking at

- splitting methods
- Eddington factors

23 Do not forget

- convergence plots

Part V

Thesis meetings

24 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)

25 Meeting on 23 September 2019

- convergence plots
- relation $N \sim \tau + \tau^2/2$
- limb darkening

26 Meeting on 30 September 2019

- discussion about x_{\min} and x_{\max}
- discussion about introduction of second line.
 - take into account the Doppler shift because you have two different frames
 - make them radially streaming (release)
 - do step for step:
 - * begin with creating a correct well
- normalized frequency: $x = \frac{\nu - \nu_0}{\nu_0} \frac{c}{v_{infty}}$
- adding other resonance frequencies, involves enlarging the frequency frame.
- about the goal of the master thesis. Making a master thesis is not doing a course where all is well-defined and *a priori* known.

Part VI

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

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