

1 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).

2 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 [5.3.4](#)).
 - finished + Ok
2. Calculate analytical solution for simplified problem in the case that $\mu = 1$ (see Section [5.3.2](#)).
 - finished + Ok + can be further studied
3. Perform convergence analysis (see Section [5.3.6](#)).

3 Overview of exercises (PART III)

1. Revisit 3D limb darkening. ϕ should be sampled between 0 and 2π (see Section [4.0.2](#)). (OK)
2. Revisit convergence analysis: adapt plot formatting and standard deviation is defined as square root of variance (see Section [5.3.6](#)). (OK)
3. Test variance reduction technique (see Section [5.3.7](#))
4. Some general considerations about the definition of specific intensity (see Section [6](#))
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 [4.0.3](#)).
6. Revisit the radial streaming approximation in `pcyg.f90` for lower optical depth (e.g. `xk0=0.5`). (see Section [5.3.2](#)).
7. What happens when you add a line (e.g. $x = 0.5 = a$)? How would you do that? (see Section [5.3.8](#))
8. Towards a mathematical description of the problem.

4 Limb darkening

4.0.1 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

$$I(\mu) = I_1(0.4 + 0.6\mu) \quad (1)$$

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  $\mu = \text{sqrt}(x)$  (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).`

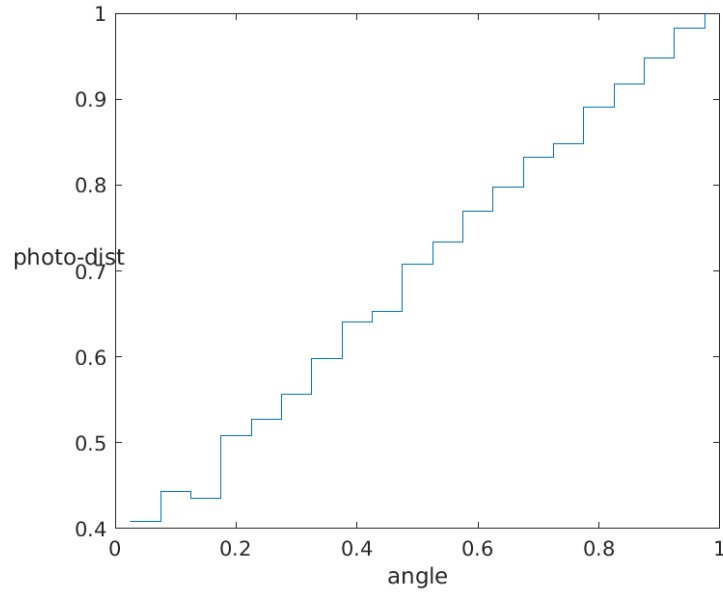


Figure 1: histogram for mu

4.0.2 3D Code

What changes is this:

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

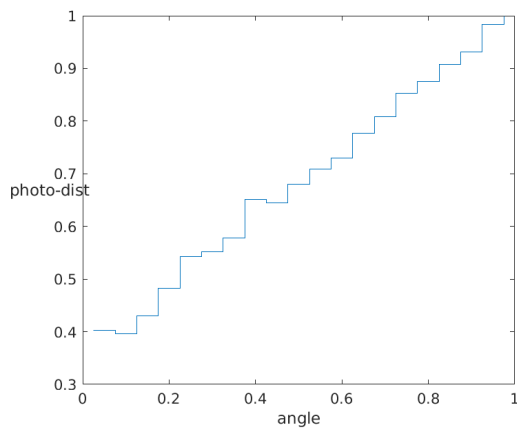


Figure 2: histogram for mu

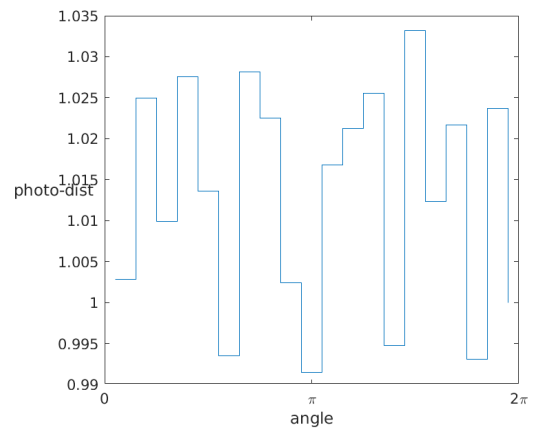


Figure 3: histogram for phi

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 3](#).

4.0.3 Closer look at Monte Carlo simulations

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 4. We observe that $N \sim \tau^2$, as can

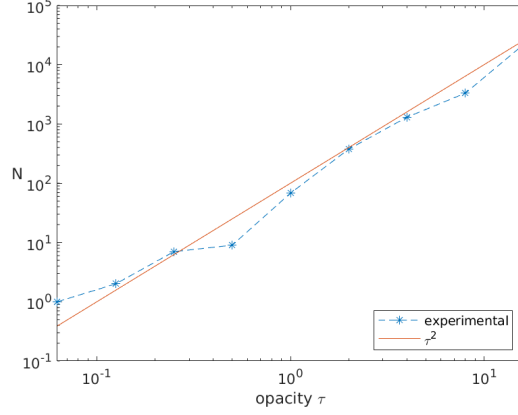


Figure 4: Number of interactions (scattering events) versus opacity, random walk

also be derived from theory.

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

$$x_N = x_{N-1} \pm l \quad (2)$$

the variance equals $\langle x_N \rangle^2 = Nl^2$

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

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

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

we have that $N = \tau^2$. This corresponds with the observations in Figure 4.

Limb darkening We first look at results from the limb darkening program. In Figure 5, the number of scattering events is plotted versus the opacity of the medium.

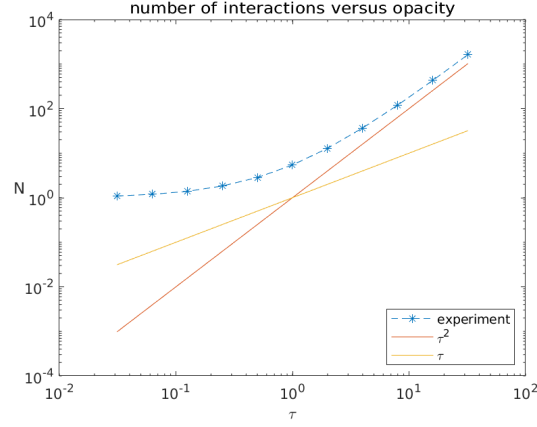


Figure 5: Number of interactions (scattering events) versus opacity, limb darkening

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

Eddington approximation

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

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

$$\mu \frac{\partial I(\tau, \mu)}{\partial \tau} = I(\tau, \mu) - J(\tau, \mu) \quad (4)$$

with the emergent intensity $I(0, \mu)$ as solution of Equation (4). Its solution equals

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

5 Investigation of program: pcyg.f90

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

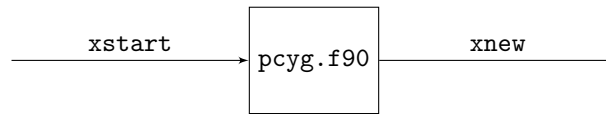
5.1 Overview of variables

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.

5.2 Mathematical things that are noteworthy

5.2.1 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 $F_\lambda = F_\nu$

5.2.2 Practical formula

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

5.2.3 Geometry & Symmetry assumptions

- spherical geometry

5.3 Exercises

5.3.1 Investigation of original code

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

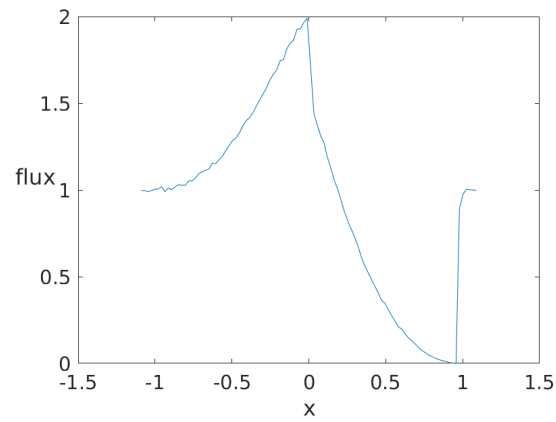


Figure 6: Original version of the code

5.3.2 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 7 for opacity `xk0 = 100`.

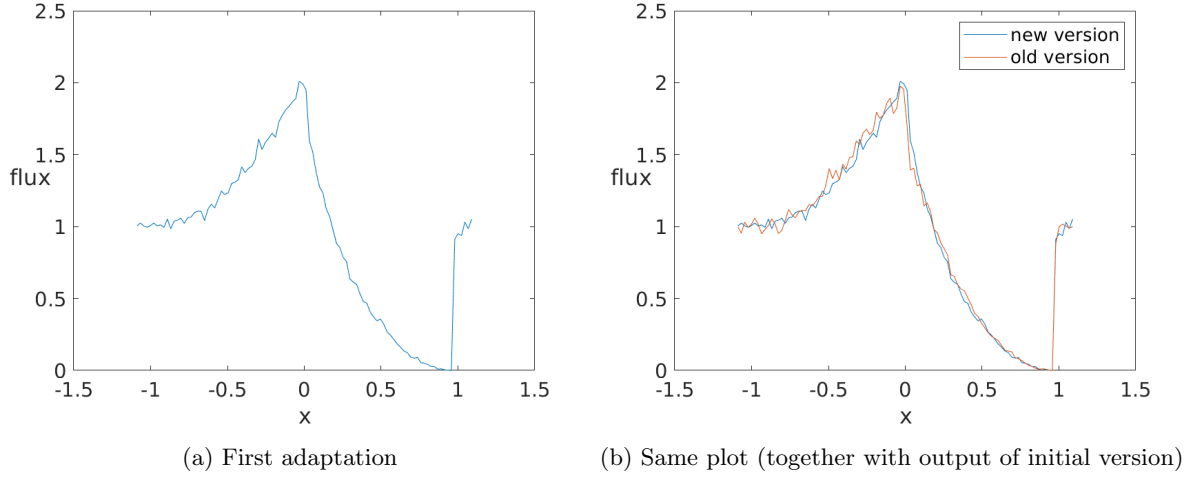


Figure 7: The number of photons equals 10^5 , `xk0=100`

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

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

$$v = v_{\infty} \left(1 - b/r\right)^{\beta} \quad (6)$$

A scaled version of Equation (6) yields

$$u = \frac{v(r)}{v_{\infty}} = \left(1 - \frac{r_{\infty}}{r}\right)^{\beta} \quad (7)$$

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

$$x_{REF} = \mu u \quad (8)$$

or thus $x_{REF} = u_{\text{interaction}}$ and than solve Equation 7 for $r_{\text{interaction}}$

- If $\mu = 1$ then

$$x = \left(1 - \frac{r_{\infty}}{r}\right)^{\beta} \quad (9)$$

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

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

$$r(x) = \frac{r_{\infty}}{1 - x^{-\beta}} \quad (10)$$

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

$$\mathbf{xmuein} = \sqrt{1 - \left[\frac{\mathbf{pstart}}{r} \right]^2} = \sqrt{1 - \left[\frac{\sqrt{1 - \mathbf{xmuestart}^2}}{r} \right]^2} \quad (11)$$

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

$$\mathbf{xmuein} = 1 \quad (12)$$

- The calculation of the optical depth goes as follows:

$$\tau = \frac{\mathbf{xk0}}{rv^{2-\alpha}(1 + \mathbf{xmuein}^2\sigma)} \quad (13)$$

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

$$\tau = \frac{\mathbf{xk0}}{rv^2(1 + \sigma)} \quad (14)$$

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

$$p(x) = \frac{1 - e^{-\tau}}{\tau} \quad (15)$$

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

$$\boxed{p(x) = \frac{1 - e^{-\frac{\tau_0}{1+x^2\sigma(x)}}}{\frac{\tau_0}{1+x^2\sigma(x)}}} \quad (16)$$

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

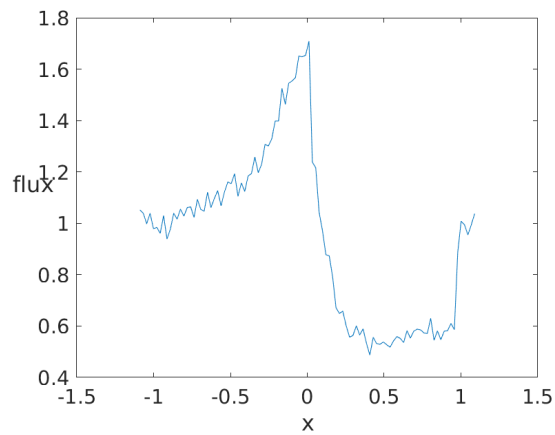
$$\mathbf{xnew} = \mathbf{xstart} + v(\mathbf{xmueou} - \mathbf{xmuein}) = \mathbf{xstart} + v(\mathbf{xmueou} - 1) \quad (17)$$

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 (17) is not applicable.

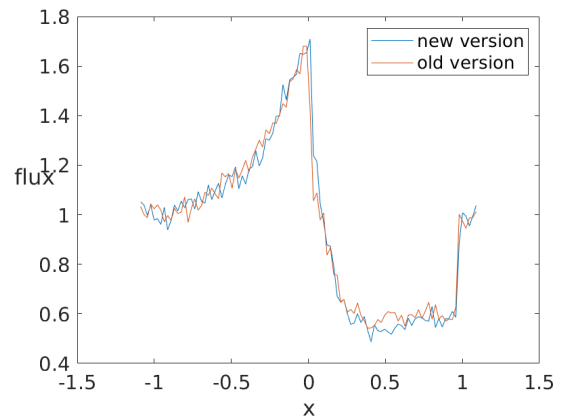
TO DO: proceed from this to the analytical expression for the flux. Here I am stuck for the moment.

Via this link, you can go back to the exercises overview: [Section 2](#).

Experiments with other opacities The results for $xk0=0.5$ are shown in Figures 8 and 9.



(a) First adaptation



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

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

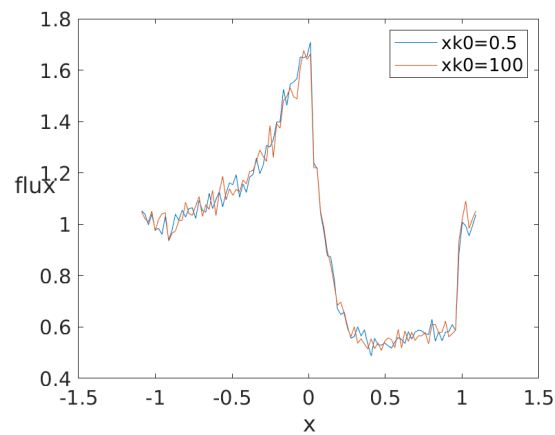


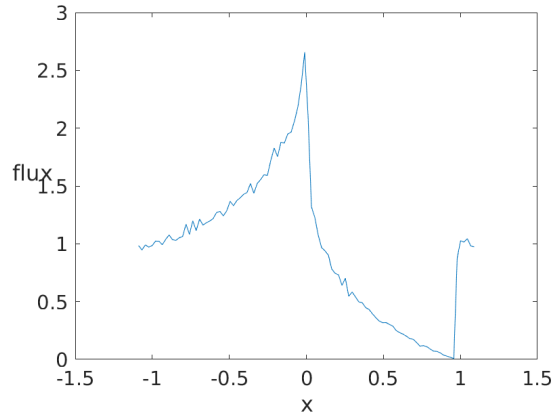
Figure 9: The number of photons equals 10^5 , $xk0=0.5$

Via this [link](#), you can go back to the exercises overview: Section 3.

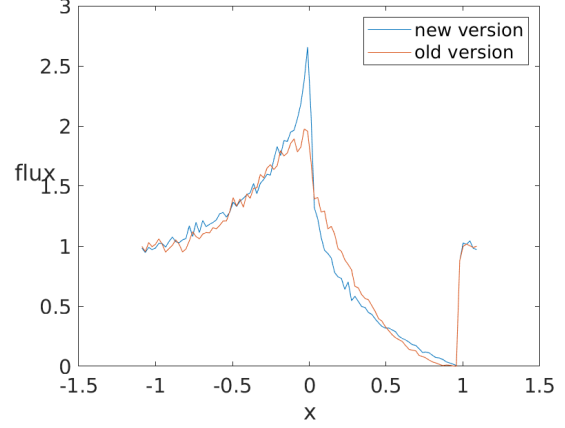
5.3.3 Second adaptation: isotropic scattering

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 10.



(a) Second adaptation



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

Figure 10: The number of photons equals 10^5

It is clear from Figure 10 that the peak around $x = 0$ is higher and sharper.

Analyse this behaviour more closely

5.3.4 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 $\frac{I(\theta)}{I(0)} = \frac{a + b \cos(\theta)}{a + b} = \frac{2}{5} + \frac{3}{5} \cos(\theta)$

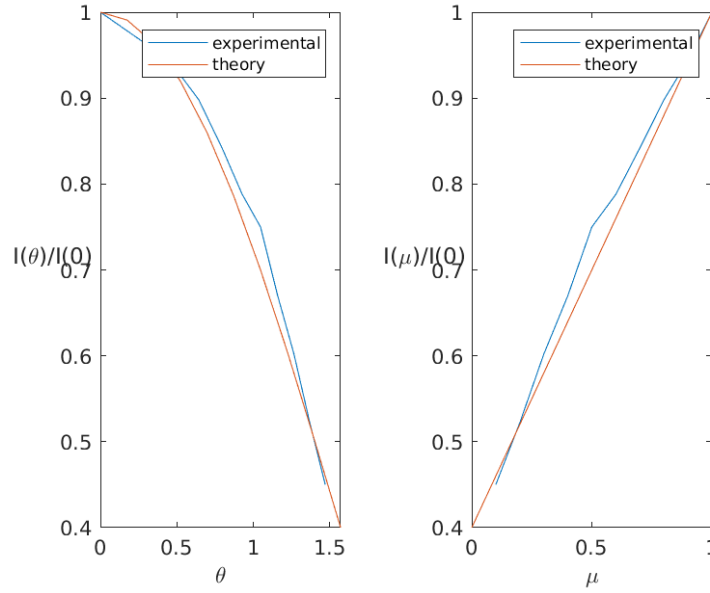


Figure 11: Eddington limb darkening (two times the same plot with $\mu = \cos(\theta)$)

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 5.3.3)

- 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

$$\xi = \int_0^\mu F_\nu d\mu = \int_0^\mu \int_\Omega I_\nu \cos(\theta) d\Omega d\mu = A \int_0^\mu \mu d\mu \quad (18)$$

together with the condition that μ satisfies a probability distribution:

$$1 = \int_{-1}^1 F_\nu d\mu = \int_{-1}^1 \int_\Omega I_\nu \cos(\theta) d\Omega d\mu = \frac{A}{2} \quad (19)$$

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

$$F_\nu = \int_{\Omega} I_\nu(0)[0.4 + 0.6 \cos(\theta)] \cos(\theta) d\Omega \quad (20)$$

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

$$\xi = \int_0^\mu F_\nu d\mu = A \int_0^\mu (0.4 + 0.6\mu) \mu d\mu \quad (21)$$

subject to the normalisation condition -very similar to Equation (19) - that

$$1 = \int_0^1 F_\nu d\mu = \frac{2A}{5} \quad (22)$$

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

$$\frac{2}{5}(0.4 + 0.6\mu) \mu d\mu \quad (23)$$

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 (23).

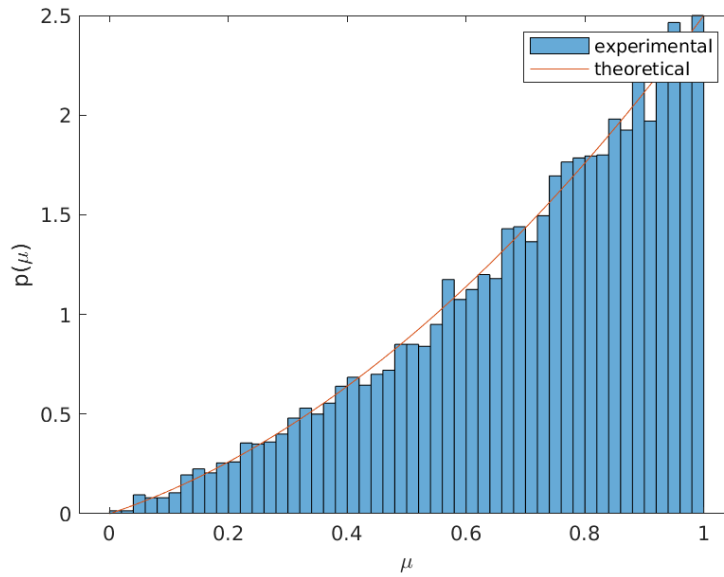


Figure 12: Accept-reject method for Eddington limb darkening

Via this link, you can go back to the exercises overview: [Section 2](#).

5.3.5 Fourth adaptaion: photospheric line-profile

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

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

5.3.6 Convergence analysis

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

kx0	alpha	beta	test_number
0	0	1	0

for a varying amount of photons, as shown in Figure 13. 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.

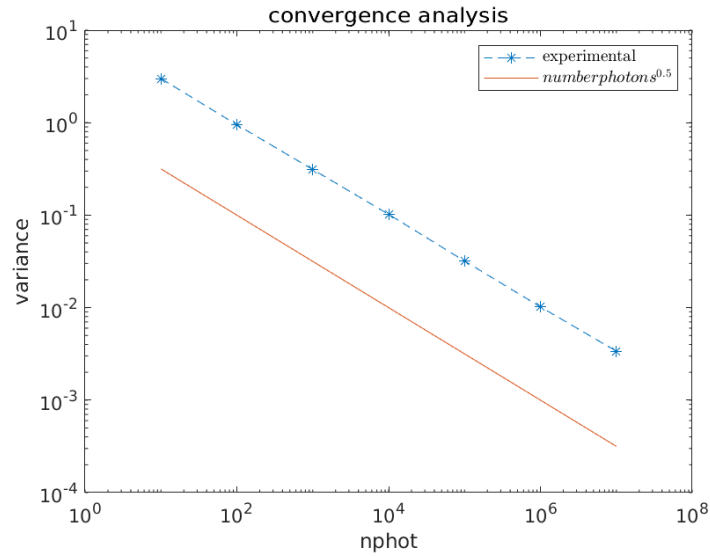


Figure 13: Original version of the code: convergence analysis (xk0=0)

Via this link, you can go back to the exercises overview: [Section 2](#).

5.3.7 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`

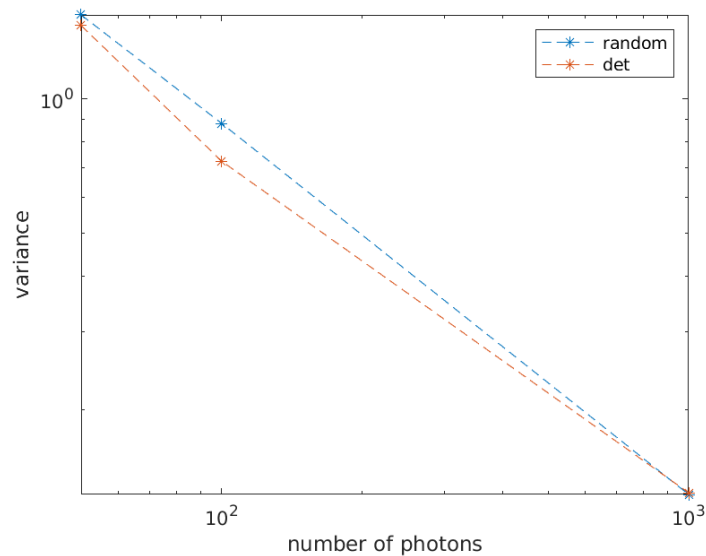


Figure 14: Original version of the code: convergence analysis ($xk0=0$)

Possible improvement: average over different stochastic realizations.

Via this link, you can go back to the exercises overview: [Section 3](#).

5.3.8 Introduction of second line

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

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 $x_{CMF} = x_{REL} - \mu\nu(r)$ 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 3 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 $x_{CMF} = x_{REL} - \mu\nu(r)$ with $x_{CMF} = 0$ and compute Sobolev optical depth
4. solve $x_{REF} = x_{CMF} - \mu\nu(r)$ 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 $x_{REF} = x_{CMF} - \mu\nu(r)$ 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

Via this link, you can go back to the exercises overview: [Section 3](#).

5.4 Mathematical description of the problem

Looking at literature

Have a look at [NoebauerUlrichM'2019MCRT].

Via this link, you can go back to the exercises overview: Section 3.

6 Definition of specific intensity

The definition of the specific intensity is

$$I_\nu = \frac{dE_\nu}{\cos(\theta)d\Omega dt d\nu d\theta} = \frac{dE_\nu}{\mu d\Omega dt d\nu d\theta} \quad (24)$$

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

$$E_\nu = N E_{\nu, \text{photon}} \quad (25)$$

To the point From this we deduce that (since, in spherical geometry $d\Omega = \sin(\theta)d\theta d\phi = d\mu d\phi$)

$$I_\nu(\mu)\mu = \frac{dE_\nu}{d\Omega dt d\nu d\theta} = \frac{dE_\nu}{\sin(\theta)d\theta d\phi dt d\nu d\theta} = \frac{dE_\nu}{d\mu d\phi dt d\nu d\theta} = \frac{N_\nu(\mu)dE_{\nu, \text{photon}}}{d\mu d\phi dt d\nu d\theta} \quad (26)$$

$$I_\nu(\mu)\mu d\mu = \frac{dE_\nu}{d\phi dt d\nu d\theta} \quad (27)$$

here is something wrong

Via this link, you can go back to the exercises overview: [Section 3](#).

7 Milic Exercises

7.1 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

8 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)

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

9.1 Goldstein-Taylor

9.2 Radiative transfer