Radiative Transfer

Lecture 01

The Physics of Star Formation

Les Houches School of Physics February 20, 2024

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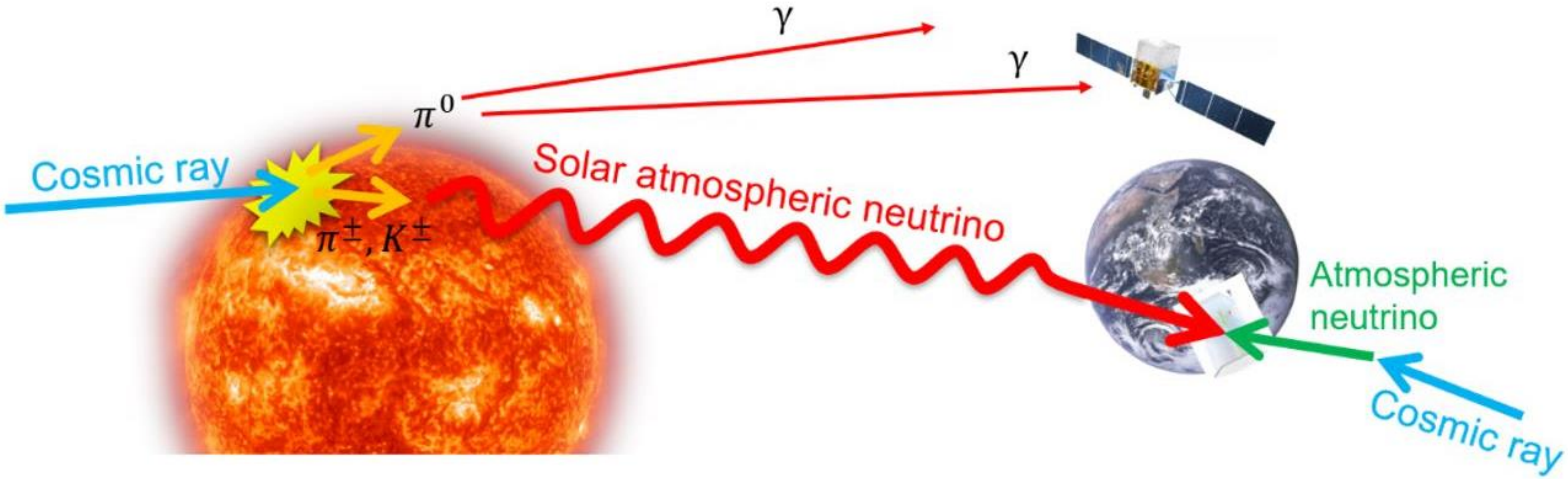
Outlook and Motivation

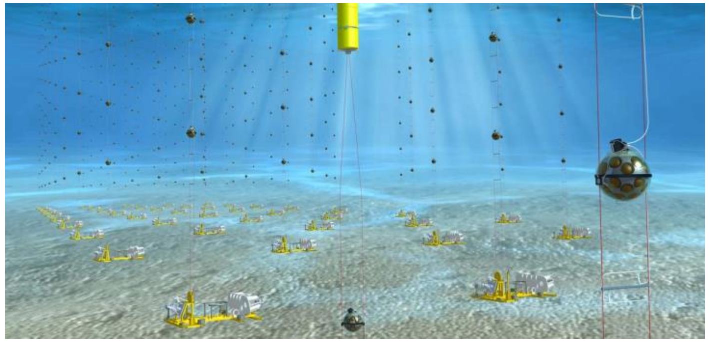
Outlook

Lecture 01:	RT Theory, RT with polarized light, Approximate solutions, Monte Carlo algorithms
Lecture 02:	optical properties of dust, more Monte Carlo algorithms, (stochastic) heating of grains
Lecture 03:	dust grain alignment dynamics, dust polarization (scattering, dichroic extinction, thermal emission), RT of polarized lines, Zeeman effect
Lecture 04:	RT of polarized synchrotron emission and Faraday rotation

Observables: Neutrinos

Supernovae, black holes, and stars generate neutrinos



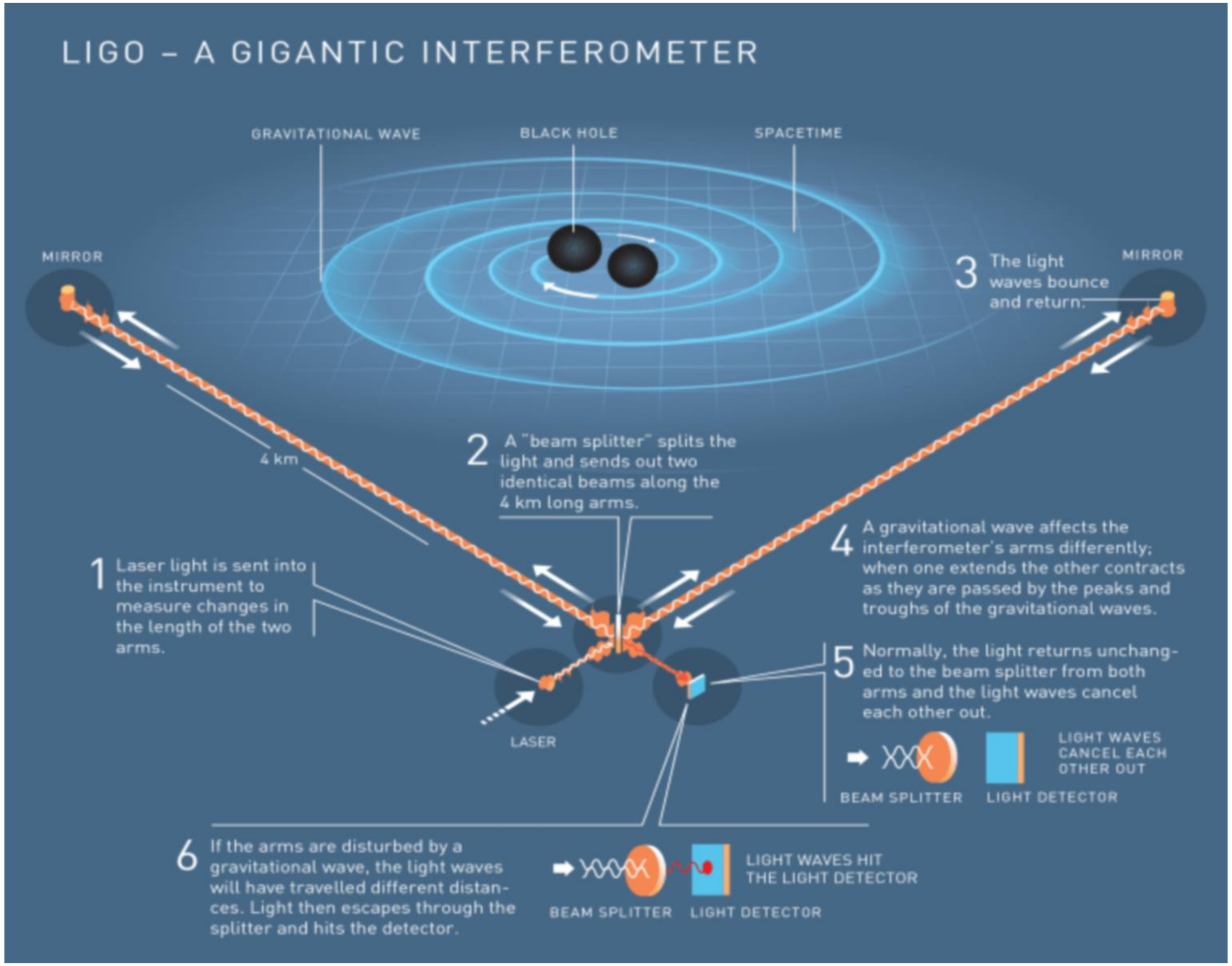


A tool to study:

- hydrogen burning (CNO cycle)
- heavy element abundance
- star core temperature
- supernova explosion mechanism,

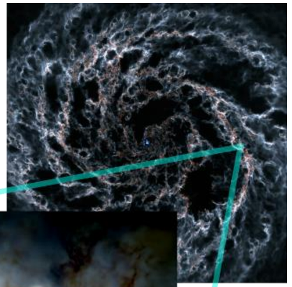
Neutrinos are hard to detect and require gigantic detectors

Observables: Gravitational waves

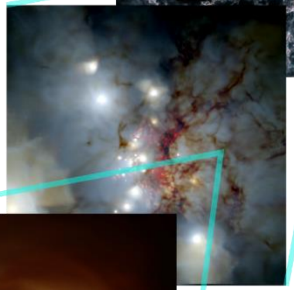


- Merging neutron stars or black holes cause minimal ripples in space-time
- Detection via large interferometers
- Allows to observe events further back into the history of our universe

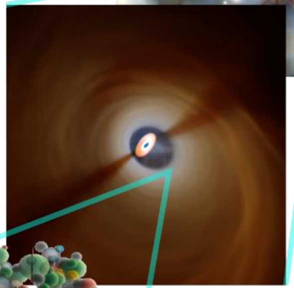
RT is a multi-scale problem



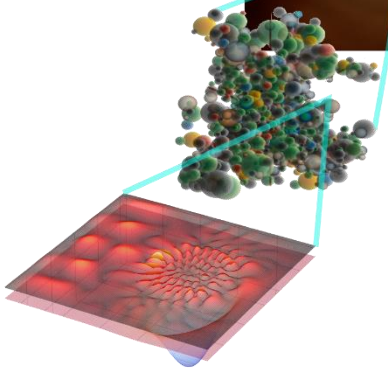
1 kly – 100 kly: Supernovae and stellar feedback shape the structure of the entire galaxy. Small dust particles are stochastically heated leading to an excess flux in some wavelengths bands. Rotating grains lead to anomalous microwave emissions



1 – 1000 ly: Dust is hiding young stars from direct observations. Polarized gives a hint about the structure of the magnetic field involved in star formation



1 – 1000 AU: Dust obscures the central star casting shows onto the outer disk. Gas and dust interactions impact heating, movement, and chemistry

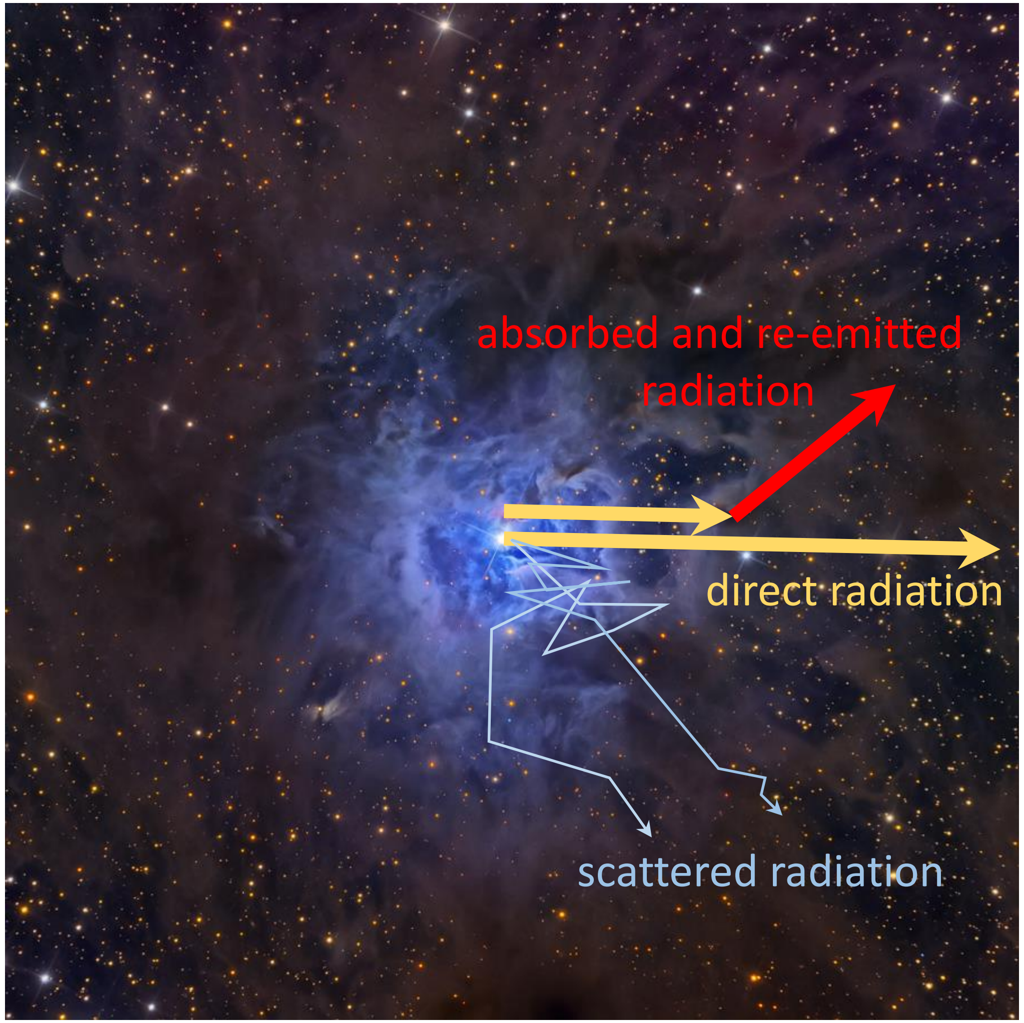


Micro- to millimeter scale: Dust grows by sticking and aggregation of smaller particles. Shapes and materials govern emission, absorption, and polarization

BUT: All we "see" in the end is light with information encoded in

1. **Intensity**
2. **Frequency / wavelength**
3. **Polarization**

RT is hard!



NGC 7023 Iris Nebula

- Multiple sources: Each star, dust grain, and gas molecule is a source emitting light in characteristic wavelengths
- Scattering: Shorter wavelength may scatter on dust several times leading to a diffusion of radiation
- Absorption: Changes the local parameters by heating and excitation of dust and gas
- Emission: Radiation is absorbed by gas and dust and re-emitted in another wavelength and direction

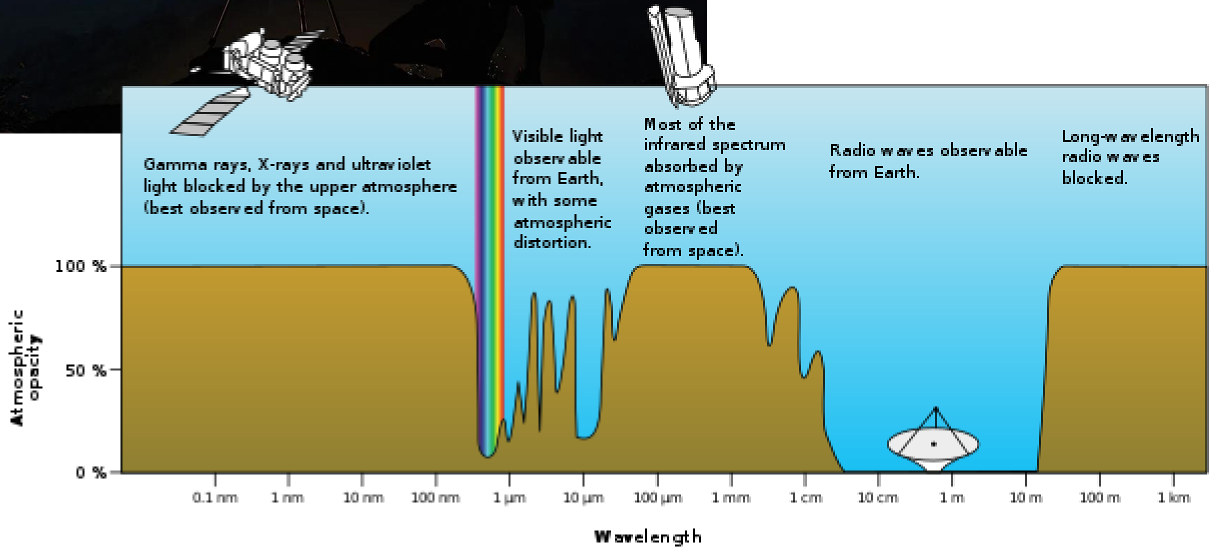
RT in astrophysics is a multi-physics, 3D, and time dependent problem and the radiation field can mostly be modeled by numerical approximations

Problems in (Radiation) Astronomy

The detection and analysis of extraterrestrial light allows to study the matter beyond your earth and solar system

Light intensity and polarization carries information:

- Emission and absorption lines: Abundance of elements, composition of dust …
- Spectral energy distribution: Gas temperature …
- Polarization: Magnetic field direction and strength …
- Line shift: Gas velocity …



Problems:

- Objects are often obscured by dust and foreground objects
- Observations are always projections of 3D information
- The earth atmosphere filters partly the incoming radiation

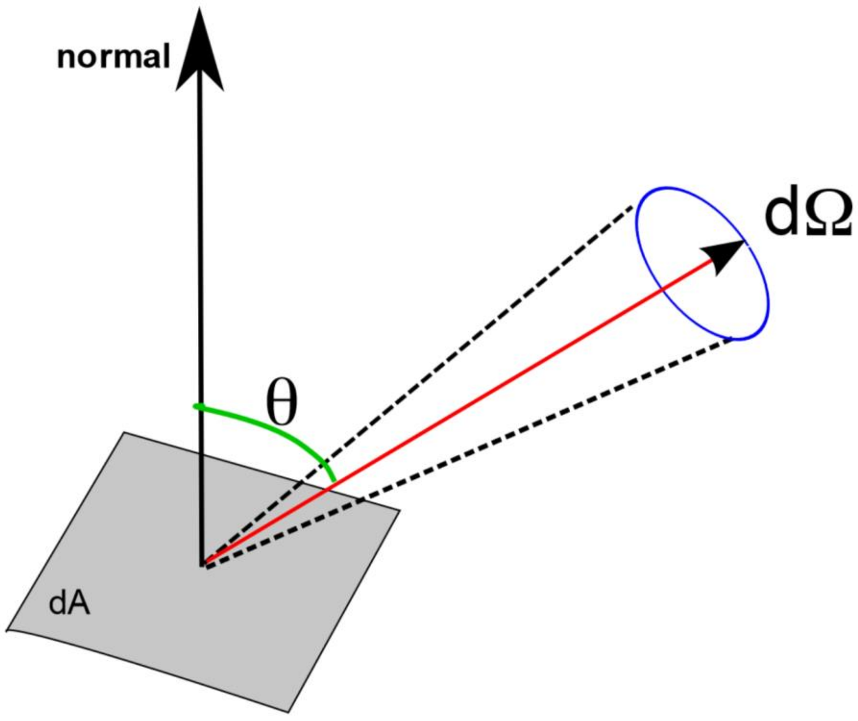
Basic RT Theory

Radiative quantities

Intensity (spectral, monochromatic) :

$$dI_\nu(\vec{r},\hat{n}) = \frac{dE}{\cos\theta \; dA \; dt \; d\Omega \; d\upsilon} \qquad [\,erg\ cm^{-1}\ s^{-1}\ \ sr^{-1}\ Hz^{-1}]$$

Note: The intensity is a scalar quantity but depends on position $\vec{r}$ and direction $\hat{n}$



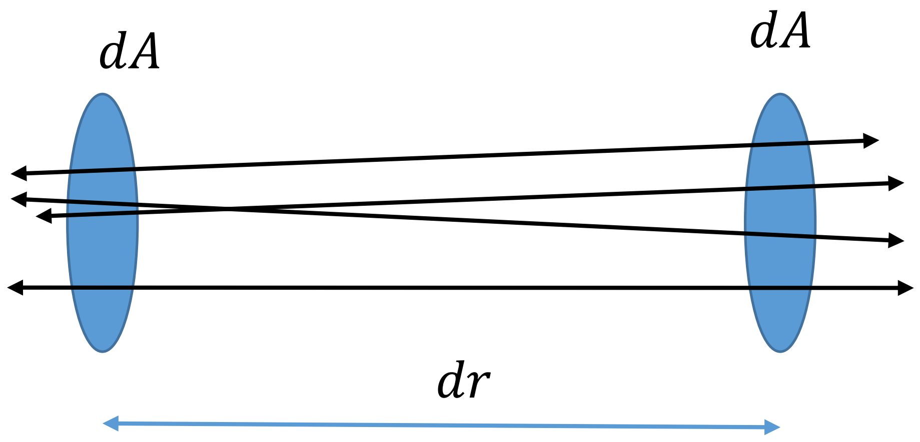
$dI_\nu = \frac{dI}{d\nu}$ per frequency

$dI_\lambda = \frac{dI}{d\lambda}$ per wavelength

$dI_E = \frac{dI}{dE} = \frac{dI}{dE}$ per energy

Where $I = \int_0^\infty I_\nu \, d\upsilon$ $[\,erg\ cm^{-1}\ s^{-1}\ \ sr^{-1}]$ is the total (bolometric) intensity

Propagation in vacuum

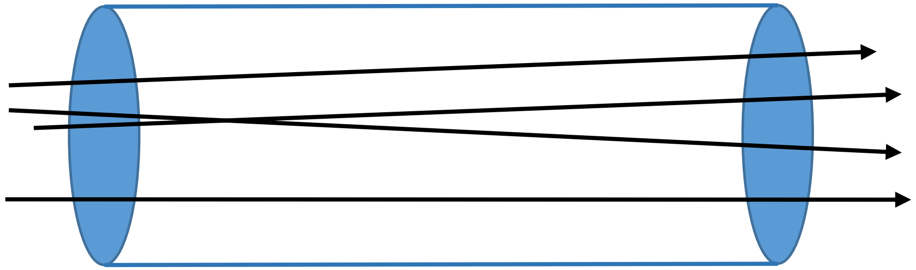


$$d\Omega_1 = \frac{dA}{dr}$$

$$d\Omega_2 = \frac{dA}{dr}$$

Consider symmetry $\Rightarrow I_1 = I_2$ i.e. $\frac{dI}{dr} = 0$

Energy density



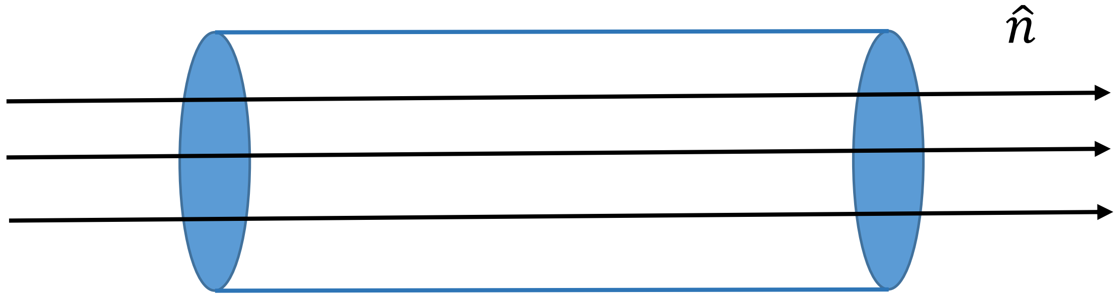
$$\frac{dE}{\cos\theta\; dV\; d\Omega} = \frac{dE}{\cos\theta\; c\; dA\; dt\; d\Omega}\,\frac{I}{c}$$

$\Rightarrow$ energy density $u = \frac{1}{c}\int_\Omega I\, d\Omega = \frac{4\pi}{c}\,\mathrm{J}\;\; [\,erg\; cm^{-3}]$

with mean intensity $\mathrm{J} = \frac{1}{4\pi}\int_\Omega I\, d\Omega\;\; [\,erg\; cm^{-1}\; s^{-1}]$

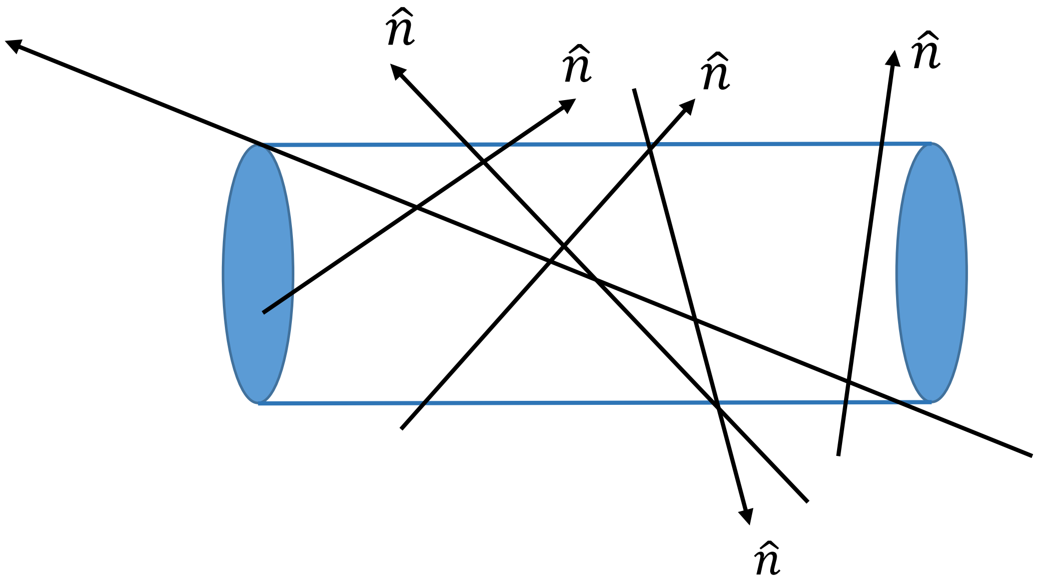
Isotropy of the radiation field

Anisotropy parameter (dimensionless): $\gamma = \frac{\left| \int_{\Omega} I\hat{n} d\Omega \right|}{\int_{\Omega} |I\hat{n}| \, d\Omega}$



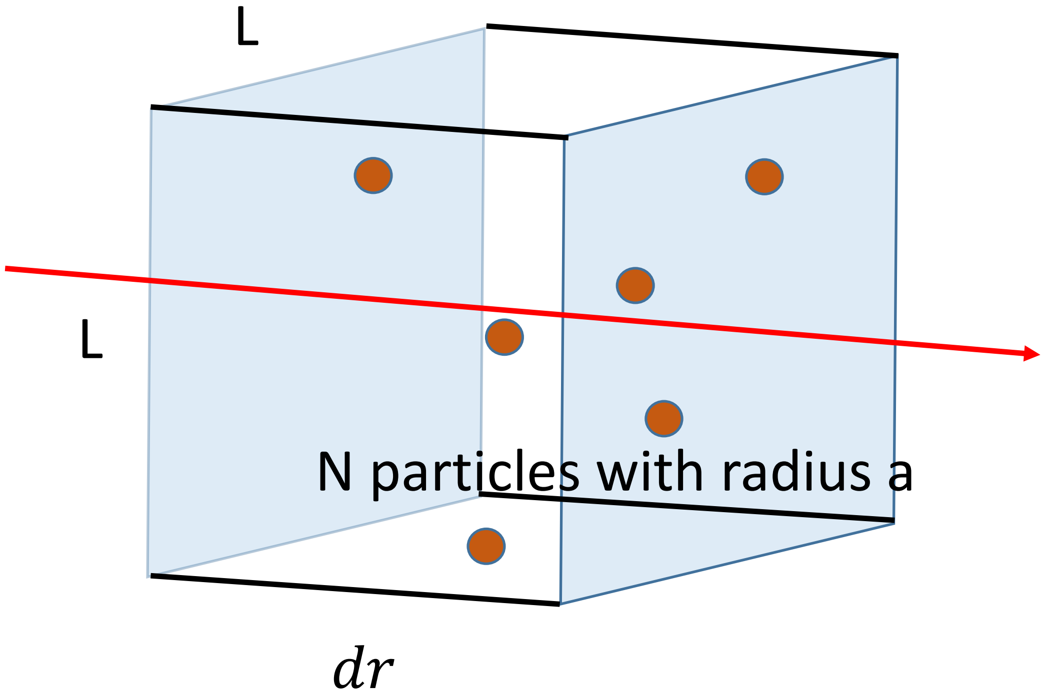
$\gamma = 1$

Note: For isotropic radiation $I = J$



$\gamma = 0$

Propagation in a medium

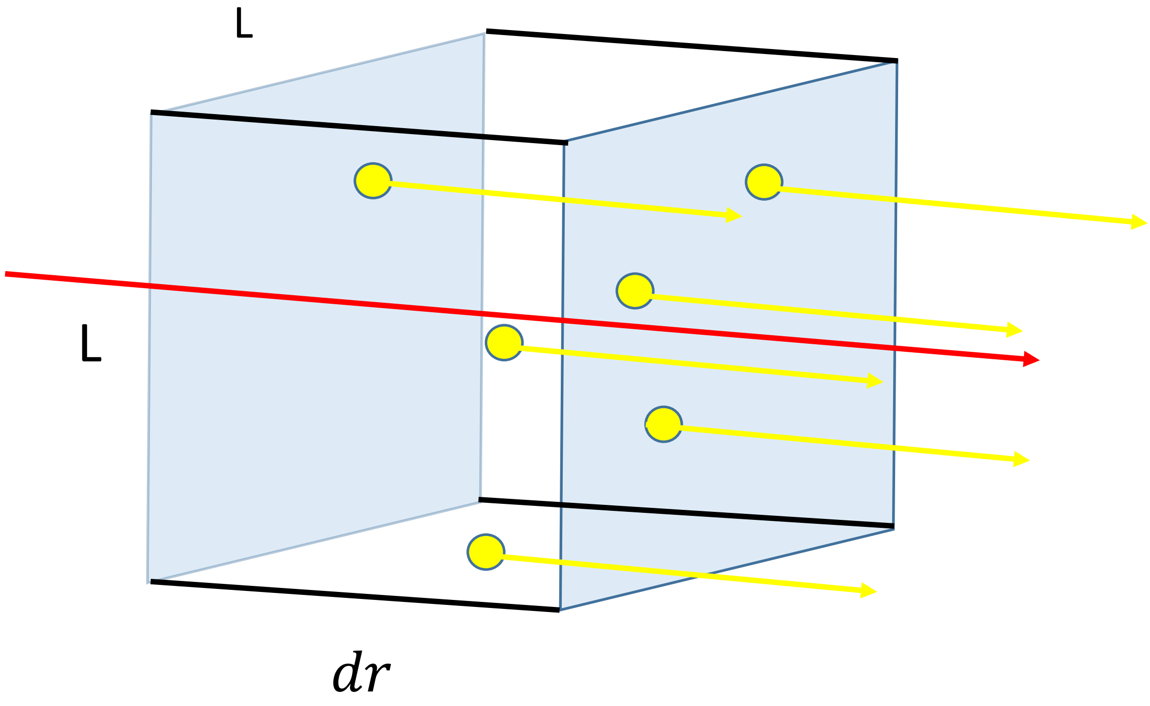


- Volume element: $V = L^2\, dr\ \ [\, cm^3]$
- Geometric cross section $\sigma = \pi a^2\, [\, cm^2]$
- Number density $n = \frac{N}{V}\ \ [\, cm^{-3}]$

Probability for a photon to "hit" a particle $\sim \frac{\text{surface of all particles}}{\text{surface of the slab}} = \frac{\sigma n L^2\, dr}{L^2} = \sigma n\, dr$

$\Rightarrow$ Light extinction (Beer–Lambert law): $\frac{dI}{dr} = -\sigma n\, I$

Light emission of the medium



Radiation can be emitted, adding energy to beam

emissivity for (spontaneous) emission

$$dj_\nu(\vec{r},\vec{n}) = \frac{dE}{dV\ dt\ d\Omega\ d\upsilon}, \quad j_\nu \propto \sigma$$

$\Rightarrow$ Change in intensity $\frac{dI}{dr} = +j_\nu$

1D monochromatic RT equation

$$\frac{dI_\nu}{dr} = -nC_\nu\, I_\nu + j_\nu$$

n: Number density [cm^{-3}]
C_ν: Cross section [cm^2]

re-written with density ρ and opacity κ_ν

$$\frac{dI_\nu}{dr} = -\rho\kappa_\nu\, I_\nu + j_\nu$$

ρ: Mass density [$g\ cm^{-3}$]
κ_ν: opacity of extinction [$cm^2\ \ g^{-1}$]

Solution to the RT problem

<u>Source function</u>

$$S_\nu = \frac{j_\nu}{\rho\kappa_\nu}$$

(in thermal equilibrium S = B_ν(T))

<u>Optical depth</u>

$$\tau_\nu = \int_0^L \rho(r)\kappa_\nu(r)\, dr$$

$$\tau_\nu = \langle\, \rho(r)\kappa_\nu(r)\rangle\, L = \frac{L}{l}$$

where l is the mean free path length of the photons

τ_ν > 1 optically thick

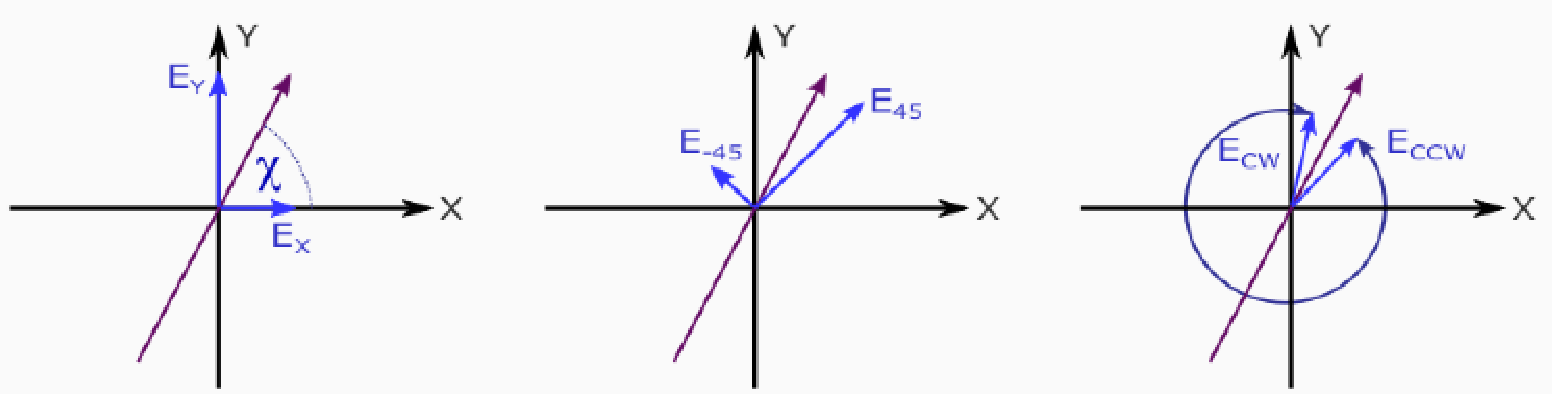
τ_ν > 1 optically thin

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)}\, S_\nu(\tau'_\nu)d\tau'_\nu$$

Are we already done?

RT with polarized radiation

Quantifying polarization



Definition: $\vec{S} = \begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} = \begin{pmatrix} E_X^2 + E_Y^2 \\ E_X^2 - E_Y^2 \\ E_{45}^2 + E_{-45}^2 \\ E_{cw}^2 - E_{ccw}^2 \end{pmatrix}$

Linear polarization: $P_l = \frac{\sqrt{Q^2 + U^2}}{I}$

Orientation angle: $\chi = \frac{1}{2} \arctan(Q/U)$

Circular polarization: $P_{circ} = {}^{V}/_{I}$

$$\frac{dI}{dr} = -\rho\kappa I + j$$

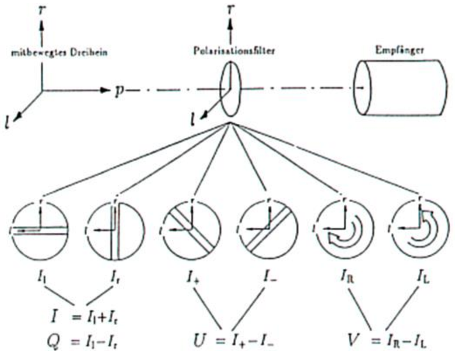
$$\Downarrow$$

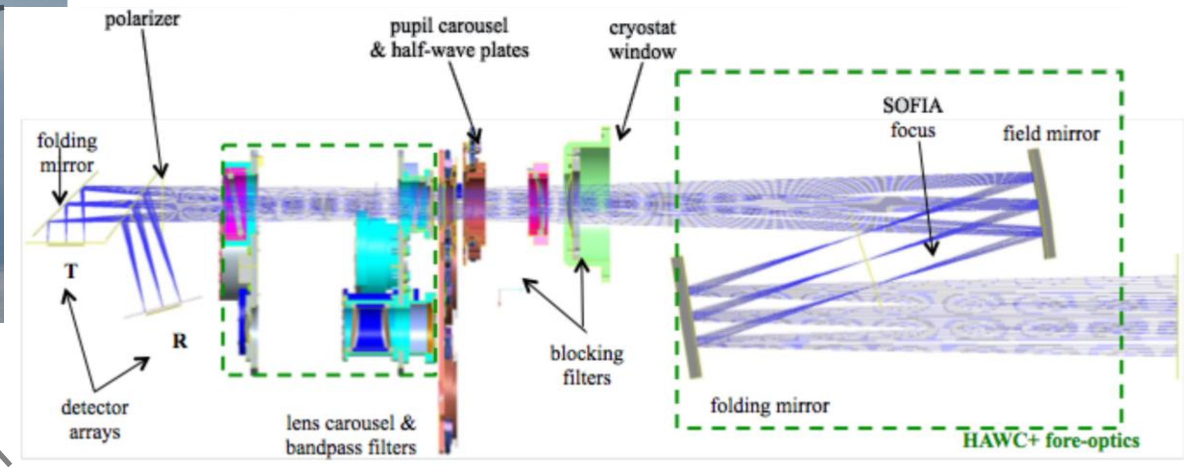
$$\frac{d\vec{S}}{dr} = -\rho\, \hat{K}\vec{S} + \vec{J}$$

where $\hat{K}$ is the 4x4 Müller Matrix and

$\vec{J} = \begin{pmatrix} j_I \\ j_Q \\ j_U \\ j_V \end{pmatrix}$ is the 4 component emissivity

Observational realization





Full Stokes vector can be constructed from four distinct positions of the half-wave plate

Choice of the coordinate system

The orientation of the coordinate system of the Stokes vector $\vec{S}$ is a free parameter!

i.e. the matrix can be transformed via $\hat{K}'=\hat{R}(\vartheta)\,\hat{K}$ with the rotation matrix

$$\hat{R}(\vartheta)=\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \cos\vartheta & \sin\vartheta & 0\\ 0 & -\sin\vartheta & \cos\vartheta & 0\\ 0 & 0 & 0 & 1\end{pmatrix}$$

Note: I and V do not rotate

For polarized dust emission e.g. exists always a rotation such that

$$\hat{K}=\begin{pmatrix}k_{11} & k_{12} & k_{13} & k_{14}\\ k_{21} & k_{22} & k_{23} & k_{24}\\ k_{31} & k_{32} & k_{33} & k_{34}\\ k_{41} & k_{42} & k_{43} & k_{44}\end{pmatrix} \rightarrow \hat{K}'=\begin{pmatrix}k_{11} & k_{12} & 0 & 0\\ -k_{12} & k_{11} & 0 & 0\\ 0 & 0 & k_{11} & k_{34}\\ 0 & 0 & -k_{34} & k_{11}\end{pmatrix}$$

Note: The matrix $\hat{K}'$ has only 3 remaining independent components!

The same for the emissivity

$$\vec{J} = \begin{pmatrix}j_I\\ j_Q\\ j_U\\ j_V\end{pmatrix} \rightarrow \vec{J}' = \begin{pmatrix}j_I\\ j_Q\\ 0\\ 0\end{pmatrix}$$

where j_U and j_V can be eliminated

Analytical solution

$$\frac{d}{dr}\begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} = -\rho \begin{pmatrix} k_{11} & k_{12} & 0 & 0 \\ -k_{12} & k_{11} & 0 & 0 \\ 0 & 0 & k_{11} & k_{34} \\ 0 & 0 & -k_{34} & k_{11} \end{pmatrix}\begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} + \begin{pmatrix} j_I \\ j_Q \\ 0 \\ 0 \end{pmatrix}$$

- Assume that the extinction and emission are constant along a length L
- Solve the upper left sub-set by substituting $A = I + Q$ and $B = I - Q$
- Solve the upper left sub-set as an eigenvalue problem

The solution is then:

- $I + Q = (I_0 + Q_0)\exp[-\rho L\ (k_{11}\text{-}k_{12})] + (j_I + j_Q)$
- $I - Q = (I_0 - Q_0)\exp[-\rho L\ (k_{11}\text{-}k_{12})] + (j_I - j_Q)$

- U = $[U_0\cos(nLk_{34}) - V_0\sin(\rho Lk_{34})]\exp[-nL\ k_{11}]$
- V = $[U_0\sin(nLk_{34}) + V_0\cos(\rho Lk_{34})]\exp[-nL\ k_{11}]$

Numerical solver

In general a numerical solution of the full set of RT equations including polarization does not exist!

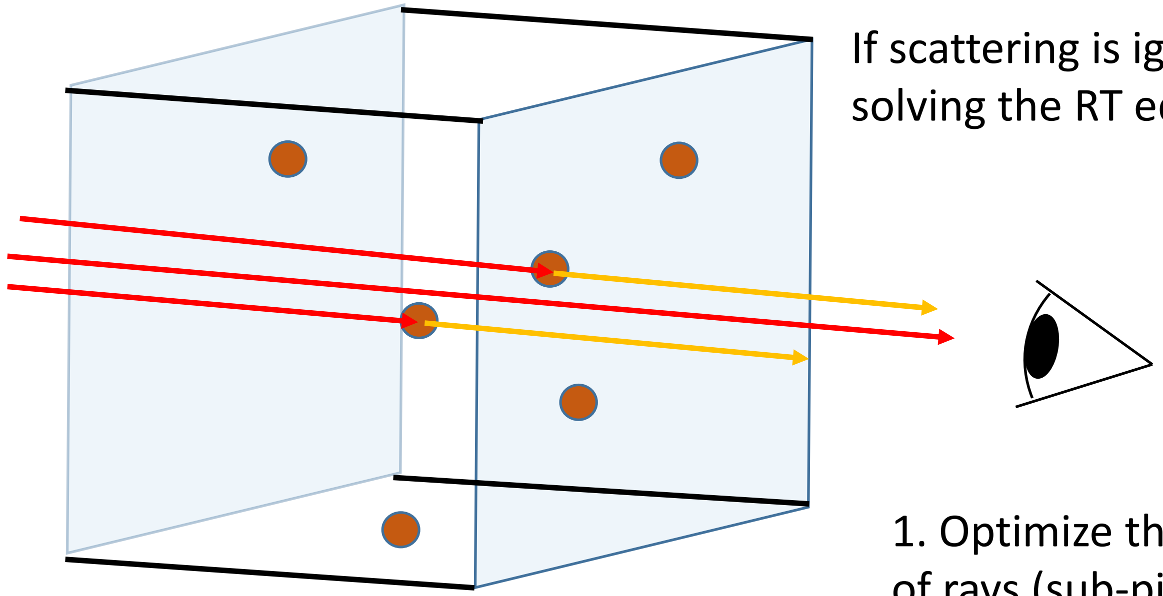
$\Rightarrow$ A solution can only ba approximated by numerical means e.g.
Runge–Kutta–Fehlberg method (RFK45):

1. Select allowed error e.g. $\varepsilon_{\mathrm{err}} = 10^{-6}$
2. Runge–Kutta solutions of the 4-th order $\vec{S}_4$ and 5-th order $\vec{S}_5$ with step size dr
3. Determine minimal error of all Stokes components $\varepsilon = \min(\varepsilon_{\mathrm{I}}, \varepsilon_{\mathrm{Q}}, \varepsilon_{\mathrm{Q}}, \varepsilon_{\mathrm{U}})$

   with $\varepsilon_{\{I,Q,U,V\}} = \left|\frac{\vec{S}_4 - \vec{S}_5}{\varepsilon_{\mathrm{err}}\vec{S}_5}\right|$

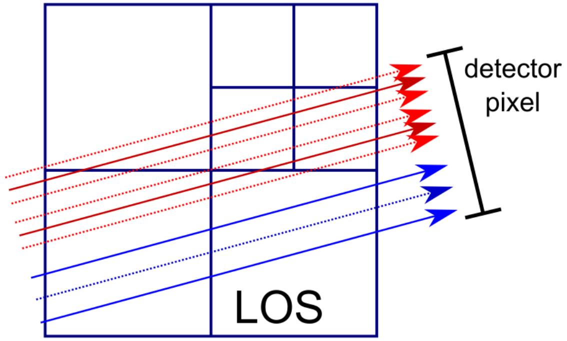
- If ε>1 select a smaller step size e.g. $dr \rightarrow 0.25\, dr\, \varepsilon^{-0.2}$
- If ε>1 select a smaller step size e.g. $dr \rightarrow 4\, dr$

Ray-tracing of images

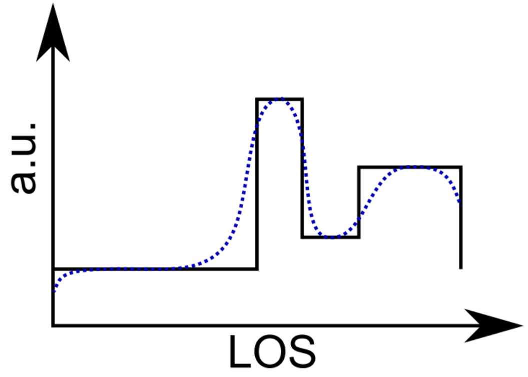


If scattering is ignored an image can be created by tracing individual rays and solving the RT equation along its line-of-sight (LOS)

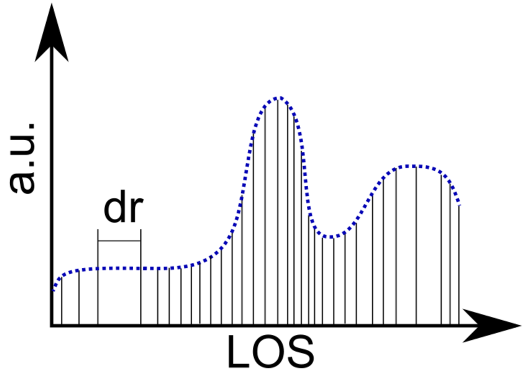
1. Optimize the umber of rays (sub-pixeling)



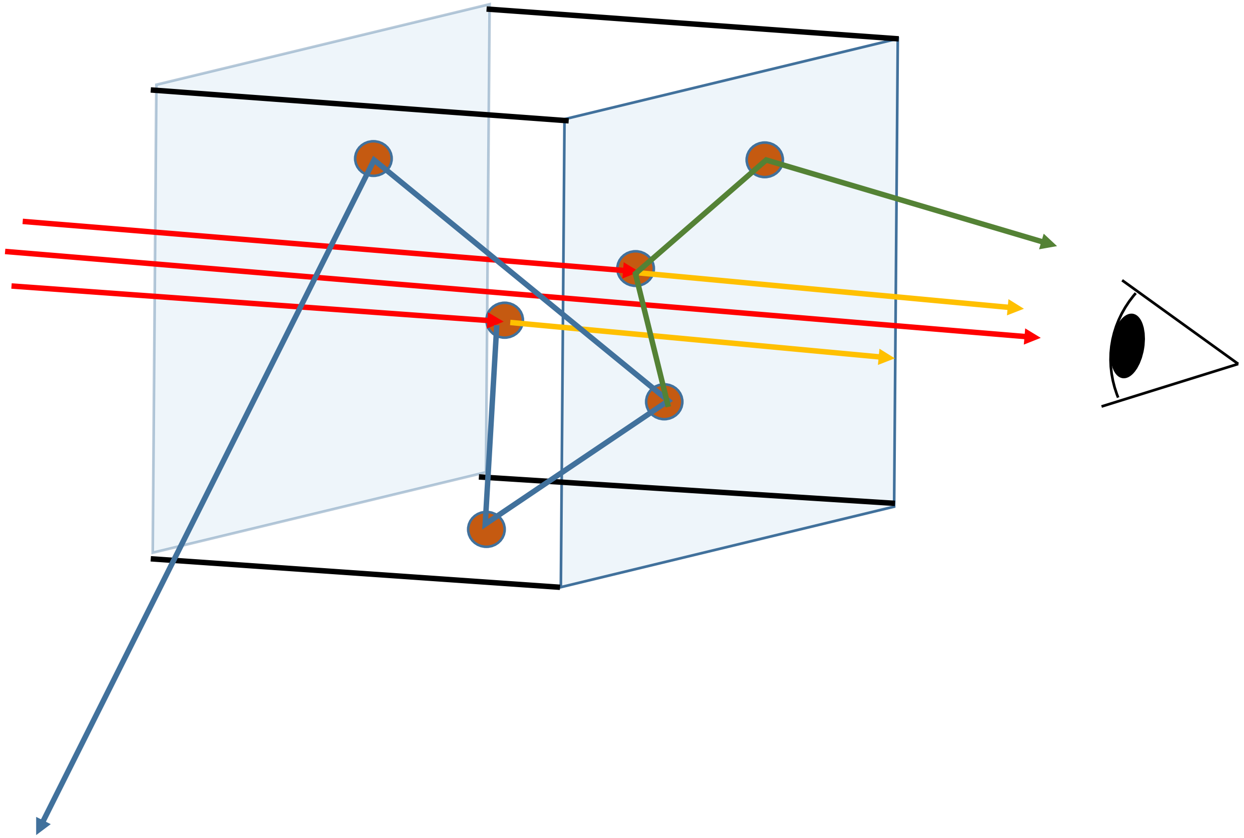
2. Interpolate between cell to allow for higher order integration



3. Solve the RT problem between individual steps dr



Scattering of radiation



$$\frac{d\vec{S}}{dr} = -\hat{K}_{abs}\vec{S} + \vec{J}_{em}$$

$$\Downarrow$$

Scattering on particles leads to an additional source $\vec{J}_{sca}$ and $\hat{K}_{sca}$ sink term

$$\frac{d\vec{S}}{dr} = -\vec{S}\left(\hat{K}_{abs} + \hat{K}_{sca}\right) + \vec{J}_{em} + \vec{J}_{sca}$$

Analytical solution and 1D integration schemes are no longer viable!

Monte Carlo MC method

Monte Carlo method

- The MC method is a set of probabilistic techniques, which all have in common that they solve equations by sampling random numbers.

- The MC method is based on random numbers but is itself not random but probabilistic!

- An algorithm samples physical quantities X from a probability density function $p(x)$ (PDF) such that the probability of finding X in an interval $[X, X + dx]$ is equal to $p(x)dx$ where $p(x)$ mimics nature.

Random number generators

An algorithm that generates a sequence of (pseudo) random numbers z distributed in the interval $z \in [0,1[$.

Demands:

- uniformly distributed in $[0,1[$
- fast and low in memory demand
- reproducibility

Examples:

Linear congruential generator:

- A sequence of number is generated by

$$y_{n+1} = (ay_n + c) \bmod m$$

- Random number $z_n = \frac{y_n}{m}$

a: multiplier
c: increment
m: modulus number
y_0: seed

KISS (Keep it Simple Stupid)

- A set of random number generators based on bit-shift operations
- Super fast with nearly no memory demand and a period of 2^{95}

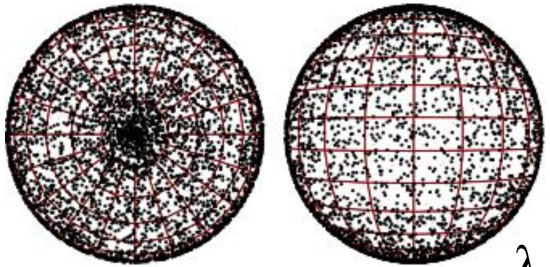
```
double getNextZ()
{
    unsigned long t;
    kiss_z = 6906969069LL * kiss_z + 1234567;

    // Xorshift
    kiss_y ^= kiss_y << 13;
    kiss_y ^= kiss_y >> 17;
    kiss_y ^= kiss_y << 43;

    // Multiply-with-carry
    t = (kiss_x << 58) + kiss_c;
    kiss_c = (kiss_x >> 6);
    kiss_x += t;
    kiss_c += (kiss_x < t);

    // Return double between 0 and 1
    return double(kiss_x + kiss_y + kiss_z) / 18446744073709551615ULL;
}
```

Monte Carlo examples

Sample random points on a sphere with equal spacing

Equal spacing in θ and φ:

- $\varphi \in [0,2\pi[\ \rightarrow \varphi_n = 2\pi\, z_n$
- $\theta \in [0,\pi[\ \rightarrow \theta_n = \pi\, z_{n+1}$



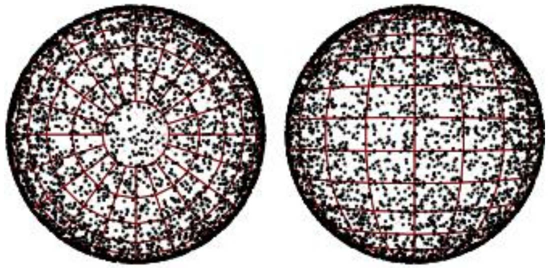
λ

Wrong way

Correct method

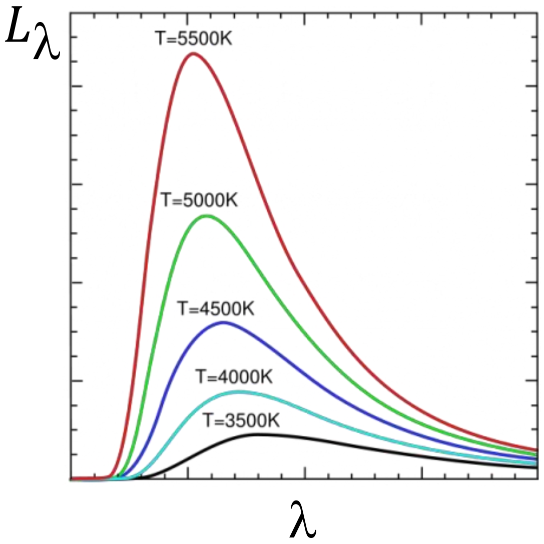
Define parameters:

- $u = 1 - 2\, z_n$
- $p = 2\pi\, z_{n+1}$
- $s = \sqrt{1 - u^2}$



unit vector $\hat{n} = \begin{pmatrix} s\ \cos p \\ s\ \sin p \\ u \end{pmatrix}$

Sample likely wavelengths of a star



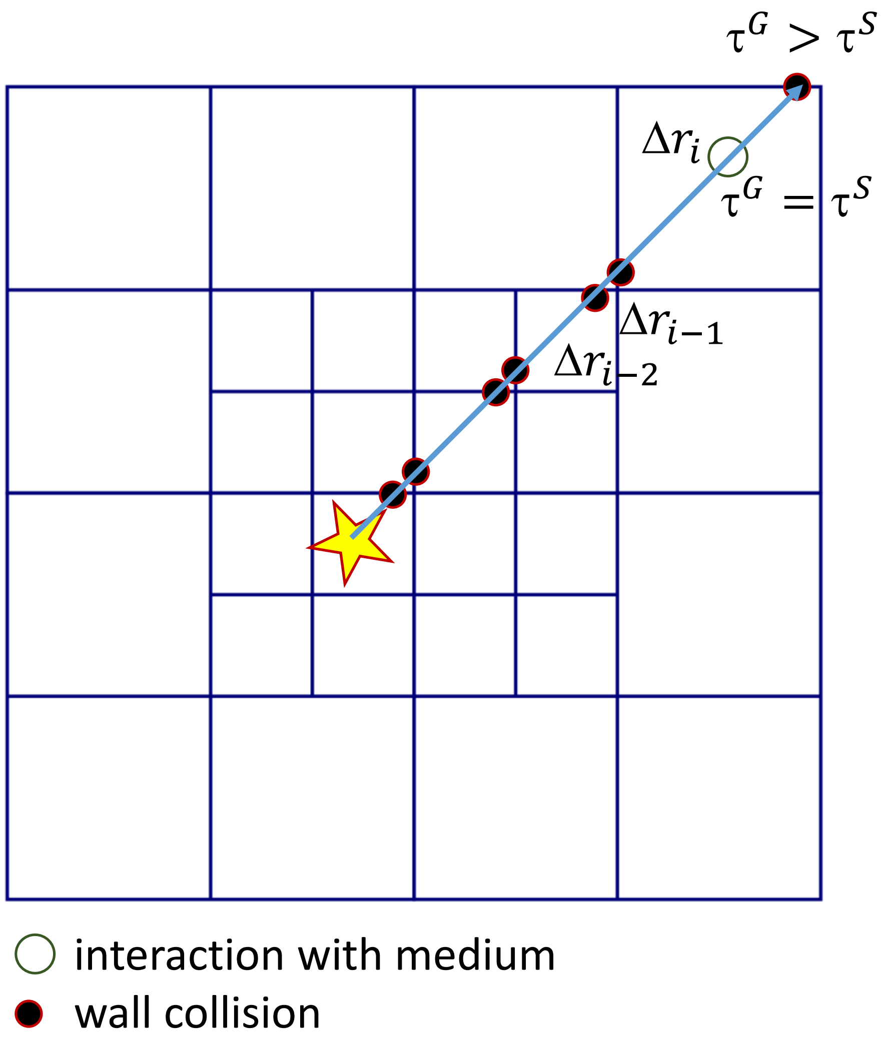
- Pre-calculate table for with

$$z_i = \frac{\int_{\lambda_i}^{\lambda_i + \Delta\lambda} L_\lambda\ d\lambda}{\int_0^\infty L_\lambda\ d\lambda}$$

Time demanding operations!

- Sample a λ e.g. from table $z_i \rightarrow \lambda_i$
- Energy per wavelengthts and unit time Δt for N_{ph} photon (packages) $\frac{\Delta E}{\Delta t} = \frac{L_\lambda}{N_{ph}}$

Simple MC RT



- Beer–Lambert law: $I = I_0 e^{-\tau}$
- Optical depth: $d\tau = \rho\kappa\, dr$

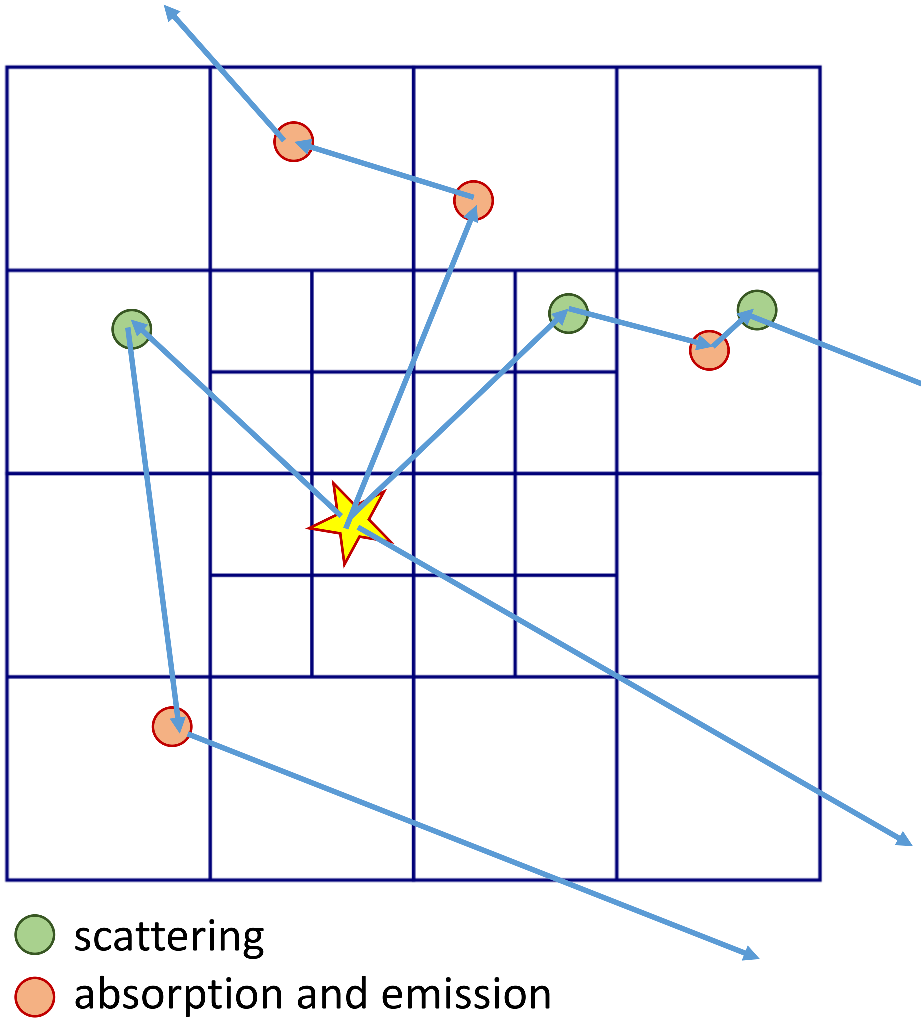
What is PDF $f(\tau)$ to “travel” a small path element dr ?

$$f(\tau)\mathrm{d}\tau = \frac{I_0 e^{-\tau}\mathrm{d}\tau}{\int_0^\infty I_0 e^{-\tau}\mathrm{d}\tau} = \frac{I_0 e^{-\tau}}{I_0}\mathrm{d}\tau = e^{-\tau}\mathrm{d}\tau$$

$\Rightarrow$ PDF $f(\tau) = e^{-\tau} \in [0,1[$
$\Rightarrow$ Distribution of optical depth can be sampled from $\tau^S = -\ln(1-z)$

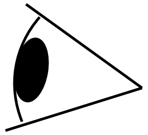
- Optical depth along path within the grid $\tau^G = \sum_i \rho_i\, \kappa_i \Delta r_i$
- Interaction with medium when $\tau^G > \tau^S$
- Re-scale last Δr_i such that $\tau^G = \tau^S$
  (sub-grid resolution)

Interaction with the medium



Define albedo $\alpha_\upsilon = \frac{\kappa_\upsilon^{sca}}{\kappa_\upsilon^{abs} + \kappa_\upsilon^{sca}}$

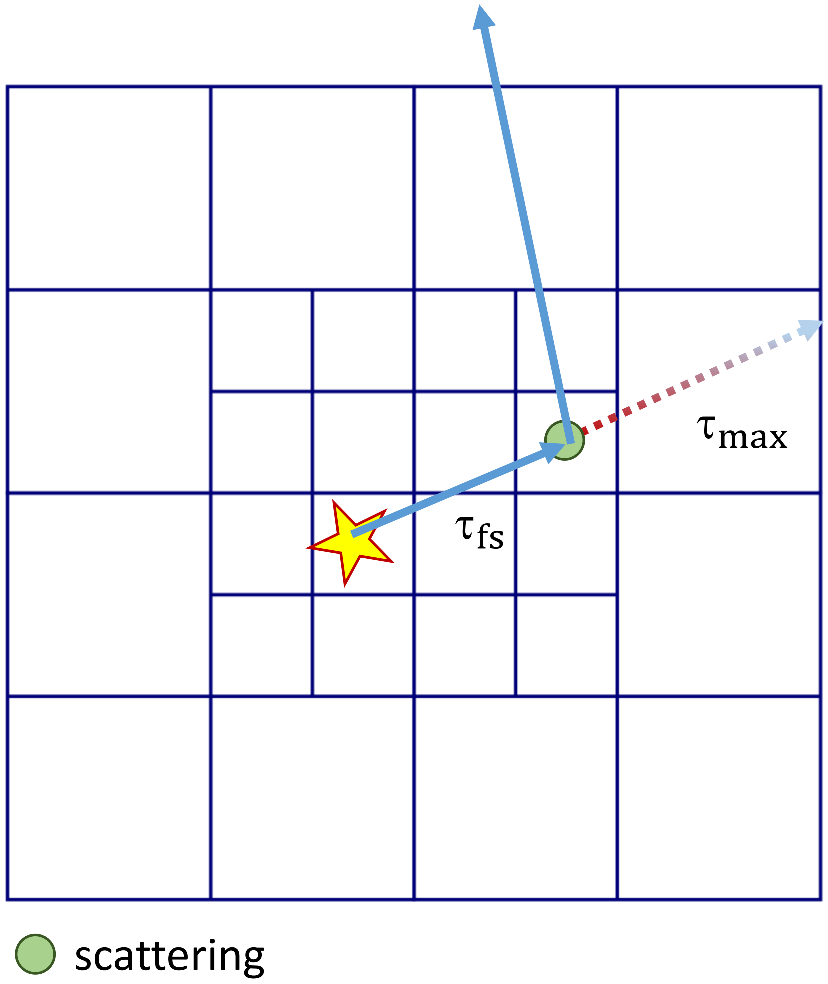
- $\alpha_\upsilon < z$ scattering event
- $\alpha_\upsilon > z$ absorption event



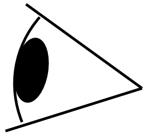
Problems with simple MC:

- Photons do not interact at all
  $\Rightarrow$ radiation field may be undetermined in same cells
- Only a few photons in direction of the observer
  $\Rightarrow$ bad signal-to-noise in the observations $\propto \frac{1}{\sqrt{N_{ph}}}$

Forced first scattering

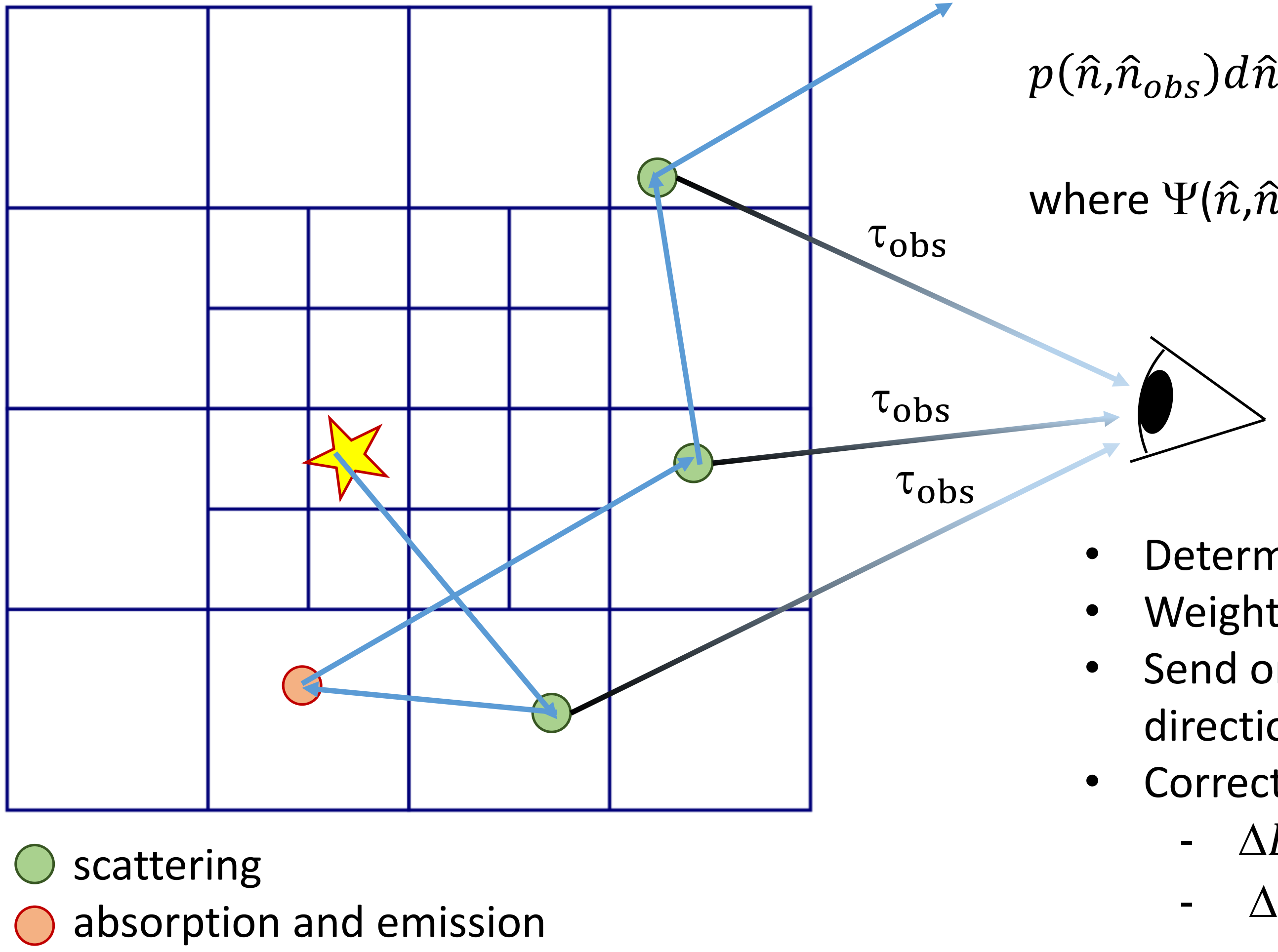


- Determine τ_{max} to the cell border
- Sample $W = 1 - e^{-\tau_{max}}$
- New optical depth is sampled from $\tau_{\mathrm{fs}} = -\ln(1 - zW)$ to guarantee at least one scattering



$\Rightarrow$ Improves diffusion of the radiation field but not the image quality

Peel-off technique



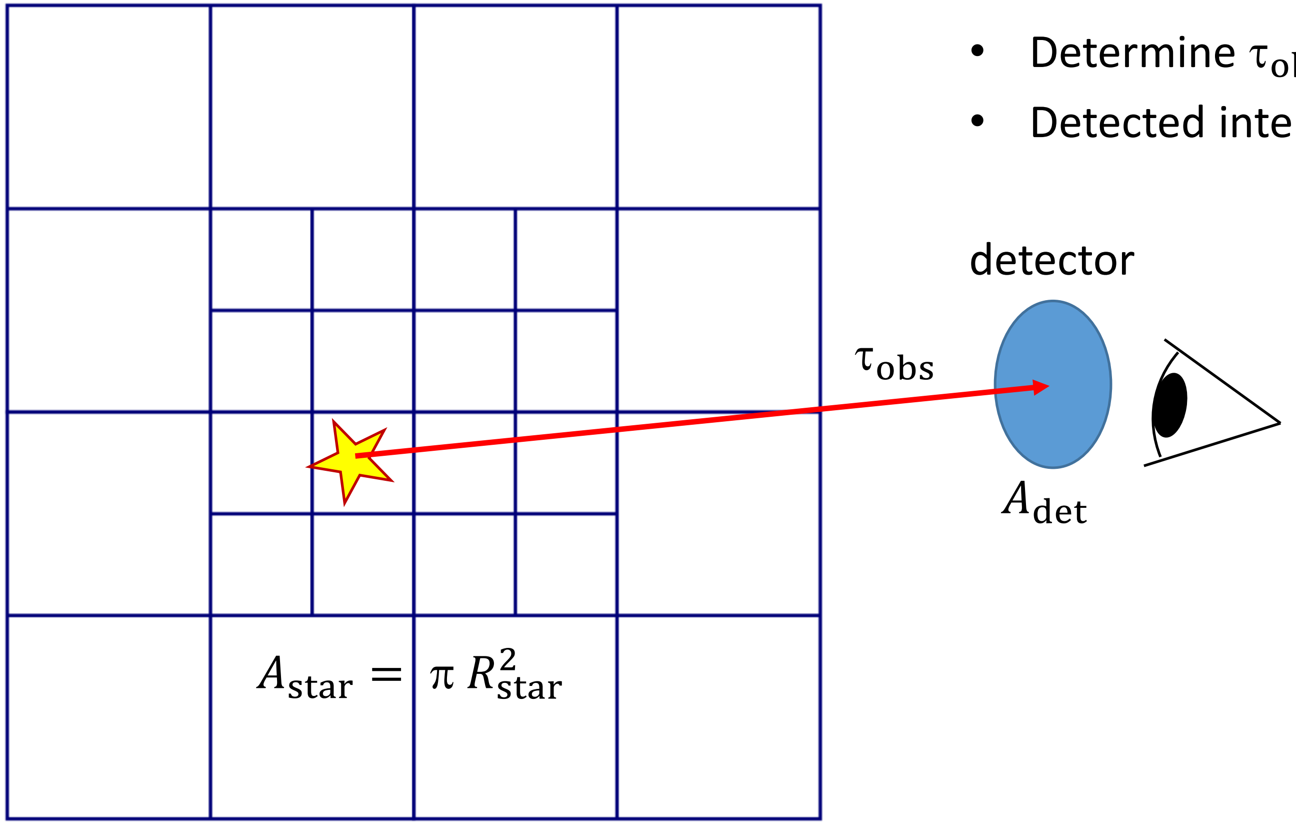
PDF $p(\hat{n},\hat{n}_{obs})$ to scatter in direction $\hat{n}_{obs}$ of the observer is

$$p(\hat{n},\hat{n}_{obs})d\hat{n}_{obs} = \frac{\Psi(\hat{n},\hat{n}_{obs})}{4\pi}\,\mathrm{d}\hat{n}_{obs}$$

where $\Psi(\hat{n},\hat{n}_{obs})$ is the scattering phase function (s. next lecture)

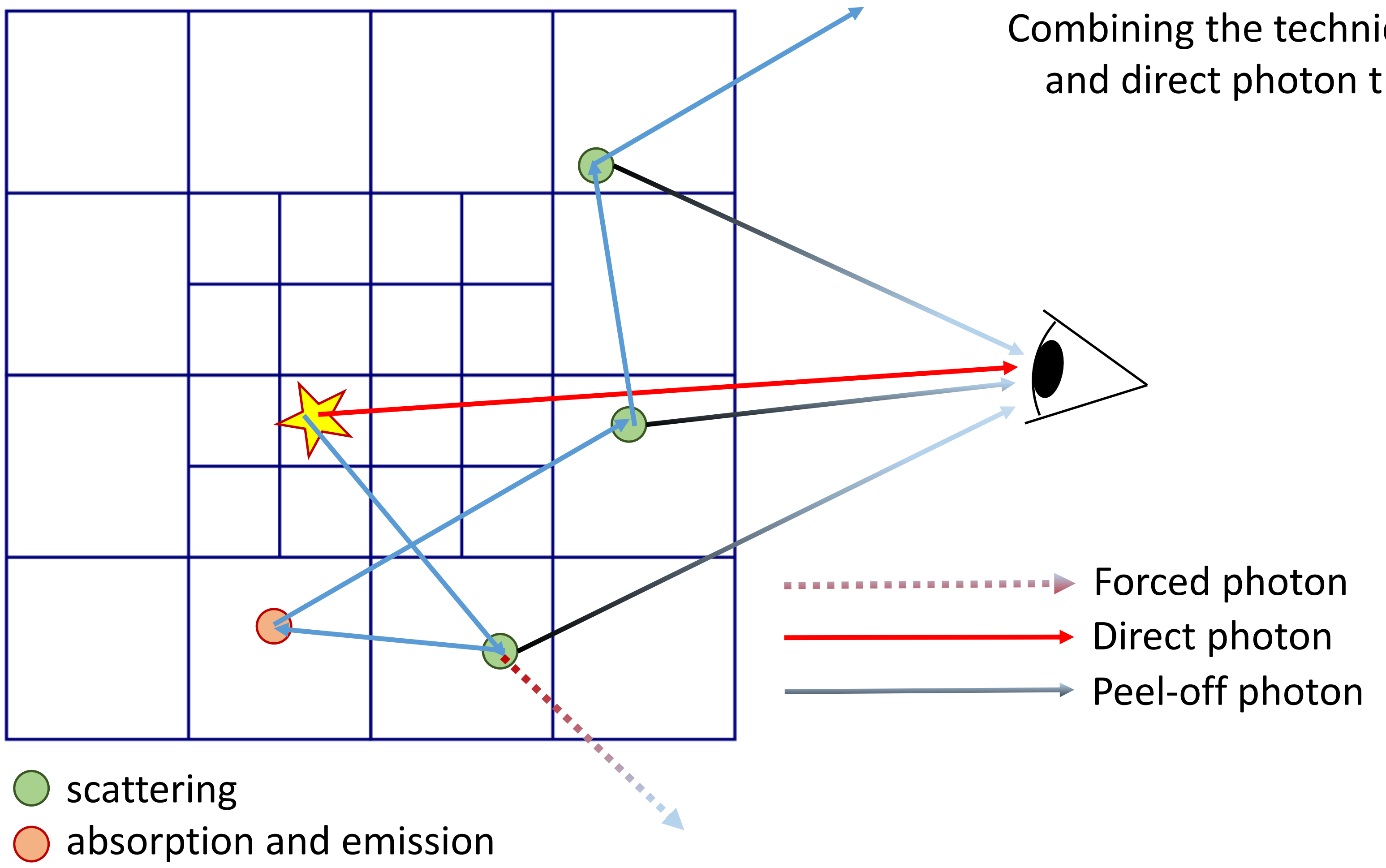
- Determine τ_{obs} from the scattering point to the observer
- Weight $W_{\mathrm{PO}} = p(\hat{n},\hat{n}_{obs})e^{-\tau_{\mathrm{obs}}}$
- Send one photon in original direction a peel-off photon in direction $\hat{n}_{obs}$
- Correct the energies between the photons:
  - $\Delta E_{\mathrm{orig}} = \Delta E\ (1 - W_{\mathrm{PO}})$
  - $\Delta E_{\mathrm{PO}} = \Delta E\ W_{\mathrm{PO}}$

Direct photon



- Determine τ_{obs} from the position of the star to the observer
- Detected intensity $I_{\mathrm{det}} \rightarrow I_{\mathrm{det}} + \frac{A_{\mathrm{star}}}{A_{\mathrm{det}}} I_{star}\, e^{-\tau_{\mathrm{obs}}}$

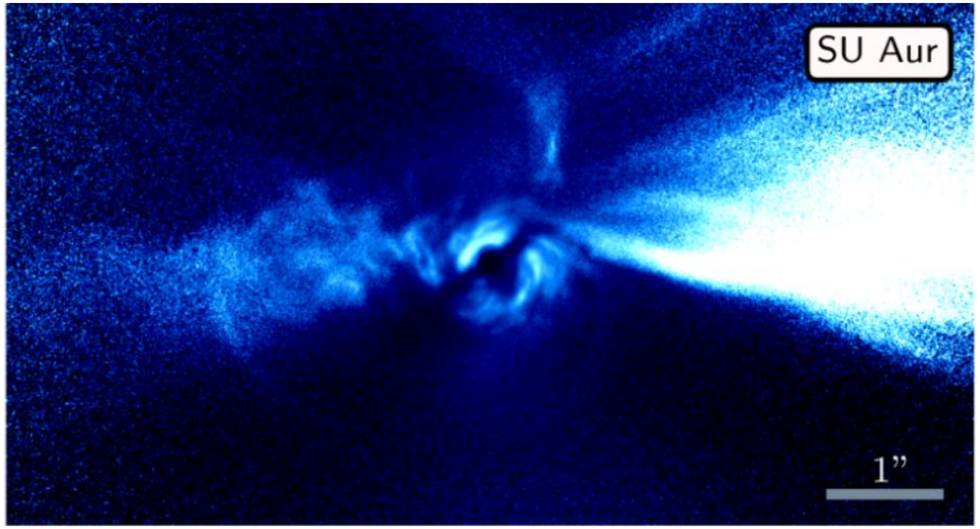
Weighted MC RT scheme



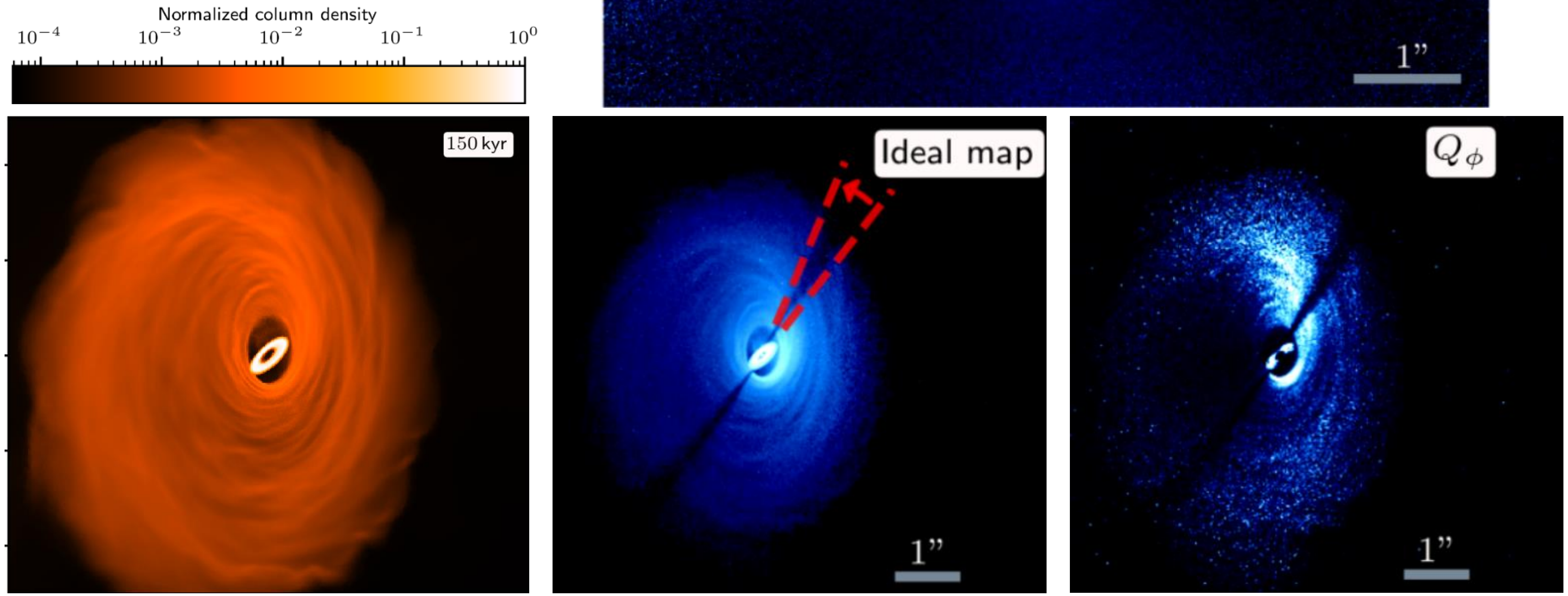
Combining the techniques of forced first scattering, peel-off, and direct photon the signal-to-noise increases “better” than $\frac{1}{\sqrt{N_{ph}}}$

RT in a dusty medium

detecting disk shadows



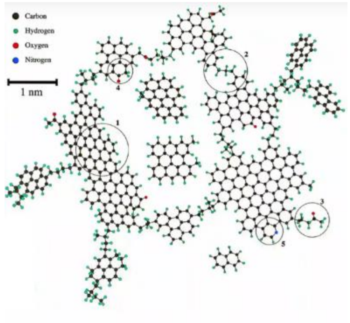
Ginsk+ 2021



Krieger+ 2024

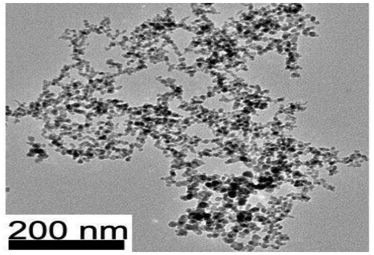
What does dust look like?

Polycyclic aromatic hydrocarbons (PAH)

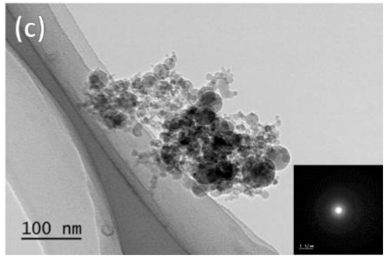


1 nm

Soot in the earth athmosphere

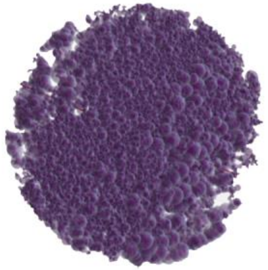


"typical" dust



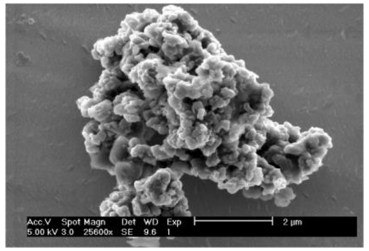
Laboratory experiment

Theoretical model



100 nm

Interplanetary dust



1 µm

meteor

1 cm

(effective) grain size: $a_{\mathrm{eff}} = \sqrt[3]{\frac{3}{4\pi} V_{\mathrm{grain}}}$

Lifecycle of dust