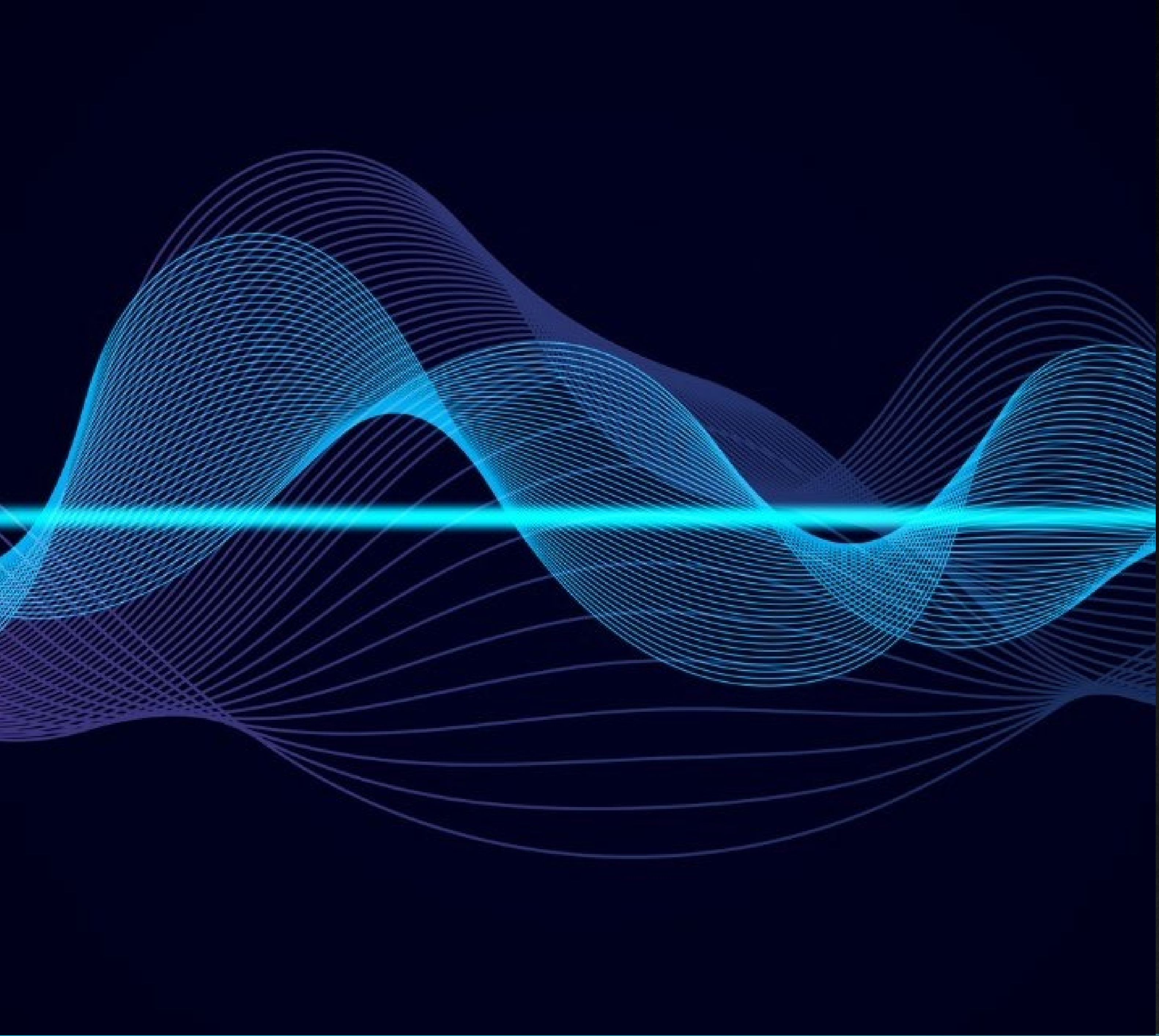


Computational Physics

PHYS 6260

Transport Methods: Photons

Announcements:

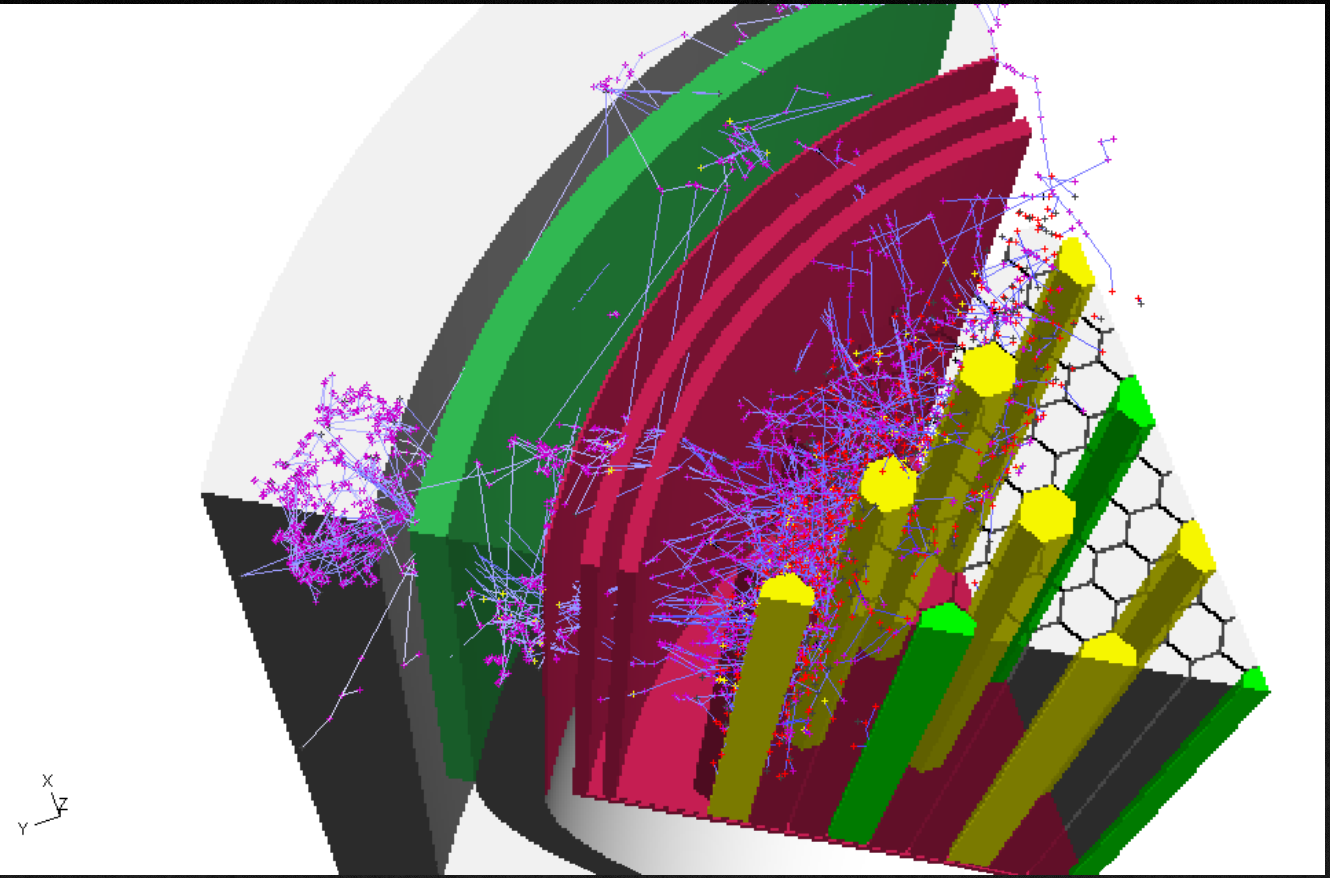
- Progress report: Due today

Lecture Outline

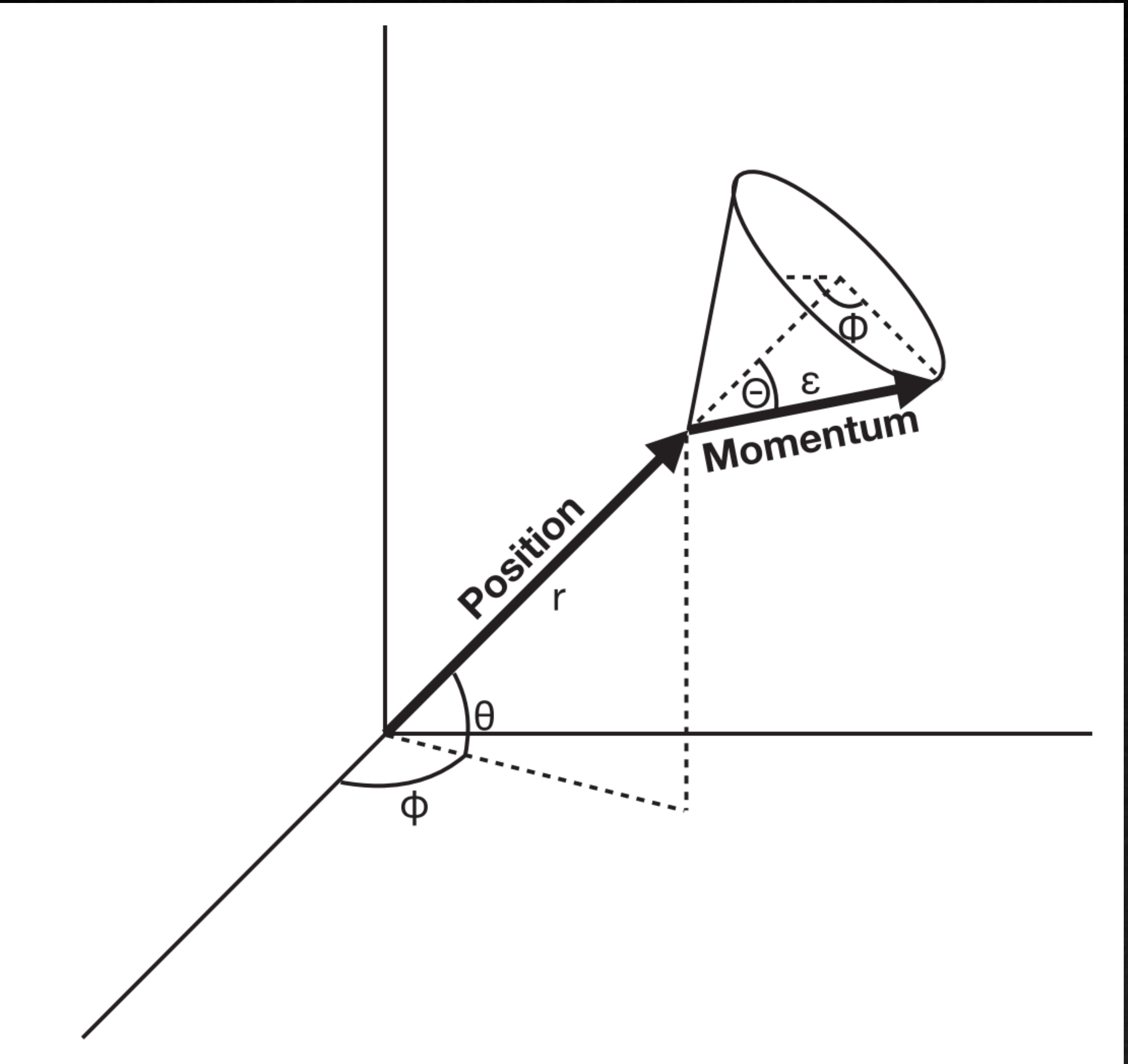
We will cover these topics

- Physics of transport
- 1D approximation
- Numerical methods for 1D transport

Physics of Transport

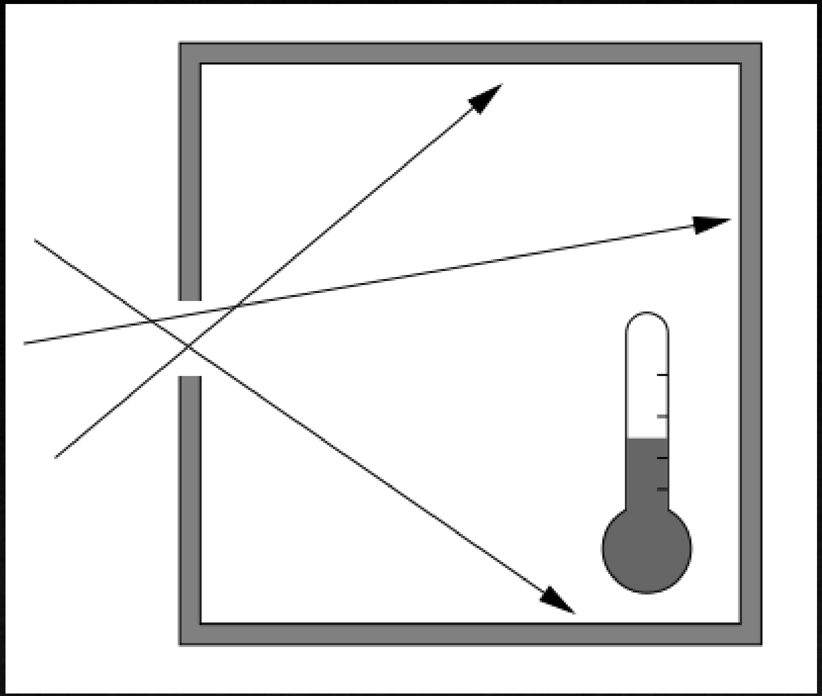


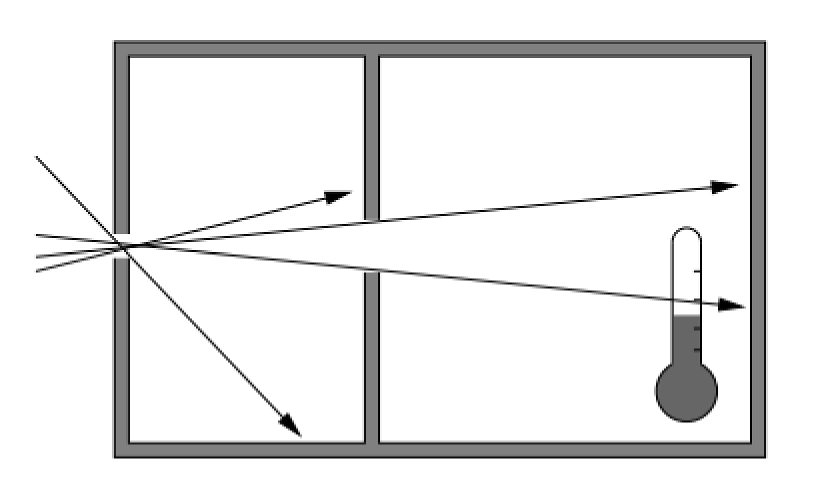
- The treatment of particle movement, scattering, absorption, production, and polarization
- Primary targets: electrons, protons, electron holes (semiconductors), neutrons, neutrinos, and photons
- Typically, the # of particles are too large to treat on a 1-to-1 basis
- Must treat as a coarsely sampled particles or as a continuous field



Transport fundamentals

- Imagine a system of particles and their momenta
- The particle flux is dependent on position, angle, energy, and time
- Seven-dimensional problem!



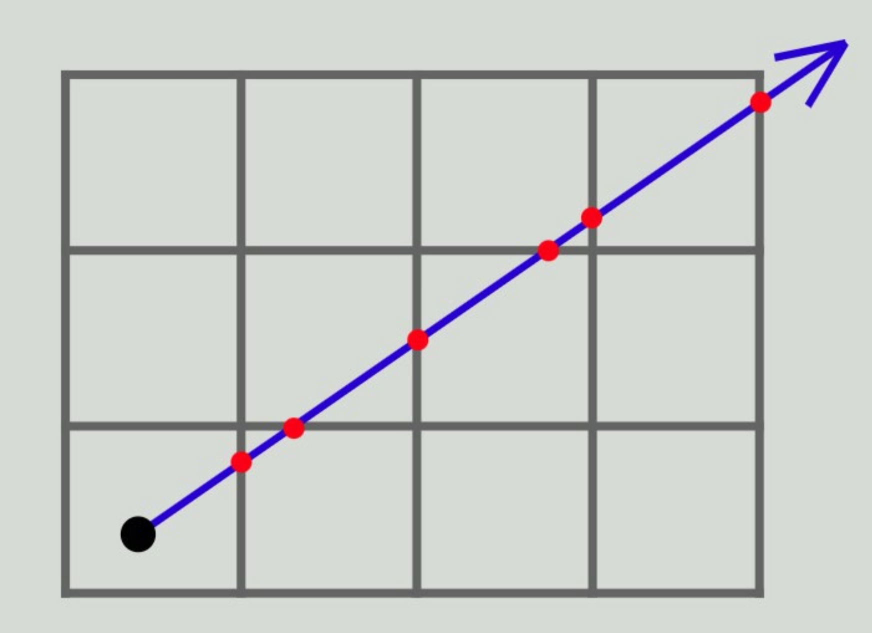


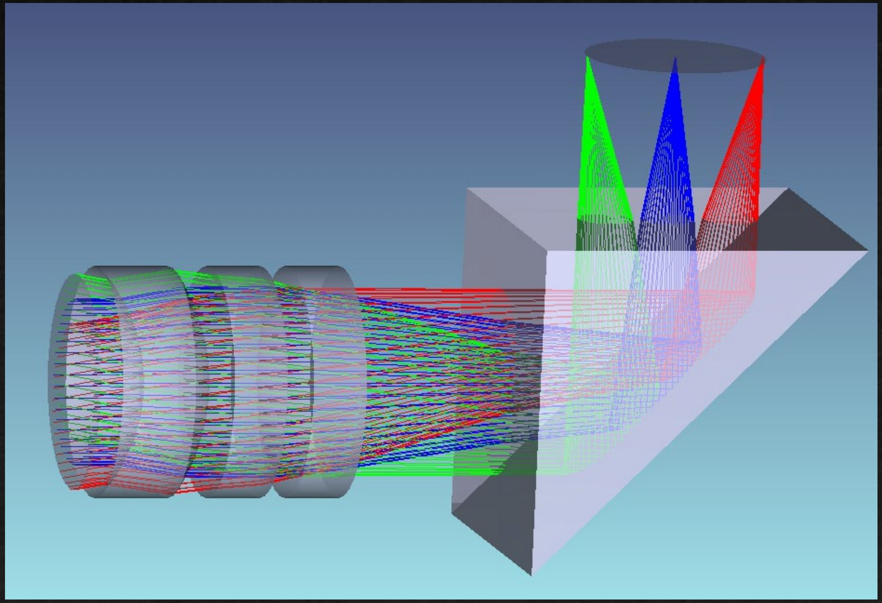
Transport fundamentals

- Flux $\vec{F}(\vec{x}, \nu, t)$: energy per time per area
- Monochromatic flux F_λ, F_ν: Flux per wavelength or frequency

$$F = \int_0^\infty F_\lambda d\lambda$$
$$\nu F_\nu = \lambda F_\lambda$$

- Intensity I, I_ν: Flux per angle
$$I(\vec{x}, \nu, \hat{n}, t) \equiv F/\Delta\Omega$$
- Radiation at some position has some directionality: $I(\vec{x}, \theta, \phi, \nu, t)$
- Convention in some fields: $\mu \equiv \cos\theta$





Transport fundamentals

- Radiation transport in one direction: ray tracing
- In vacuum, the intensity is constant

$$\hat{n} \cdot \nabla I_\nu(\vec{x}, \hat{n}) = 0$$

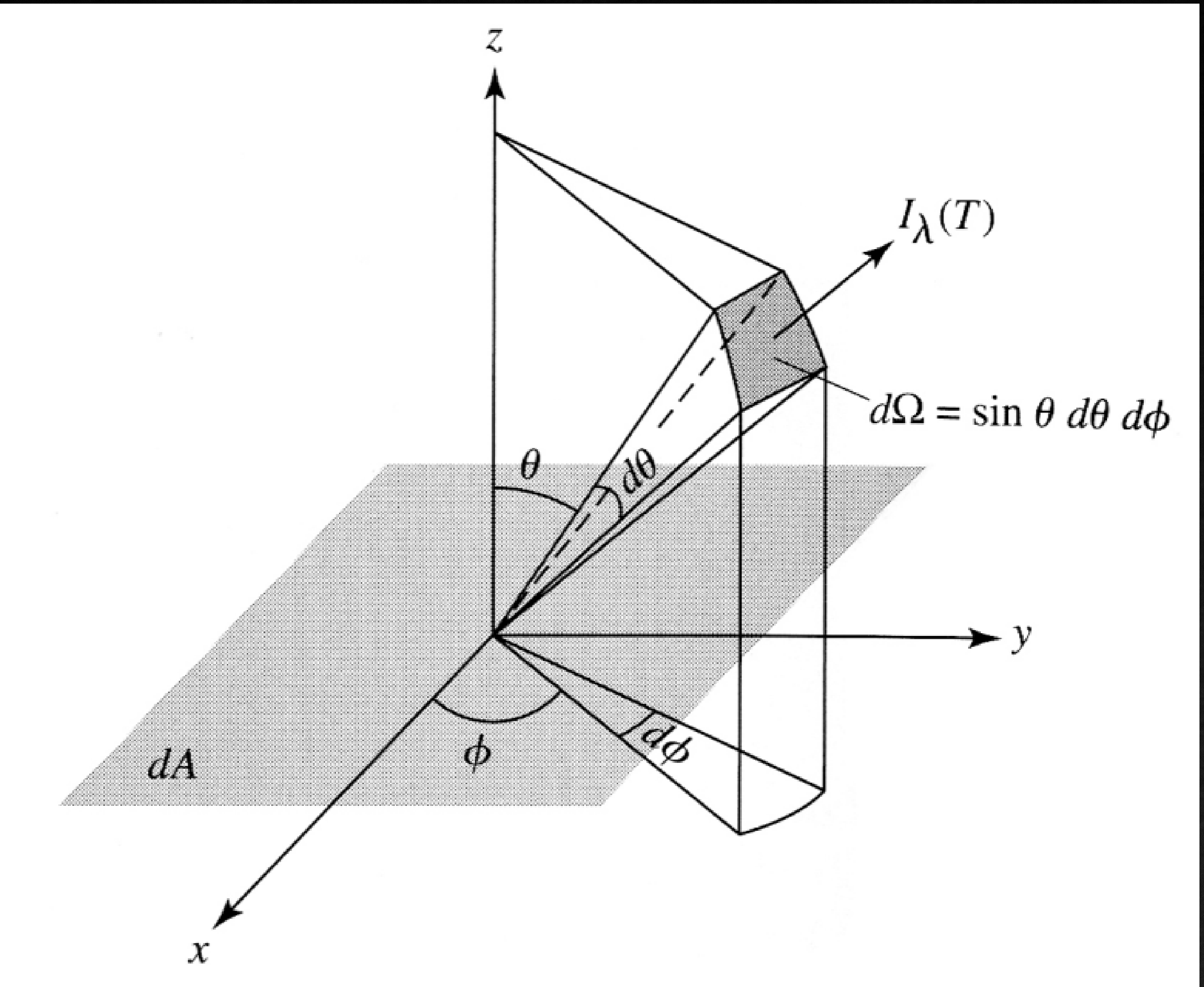
- We can write this as a differential equation along the ray

$$\frac{dI_\nu(\hat{n})}{ds} = 0$$

- where the ray's position is described as

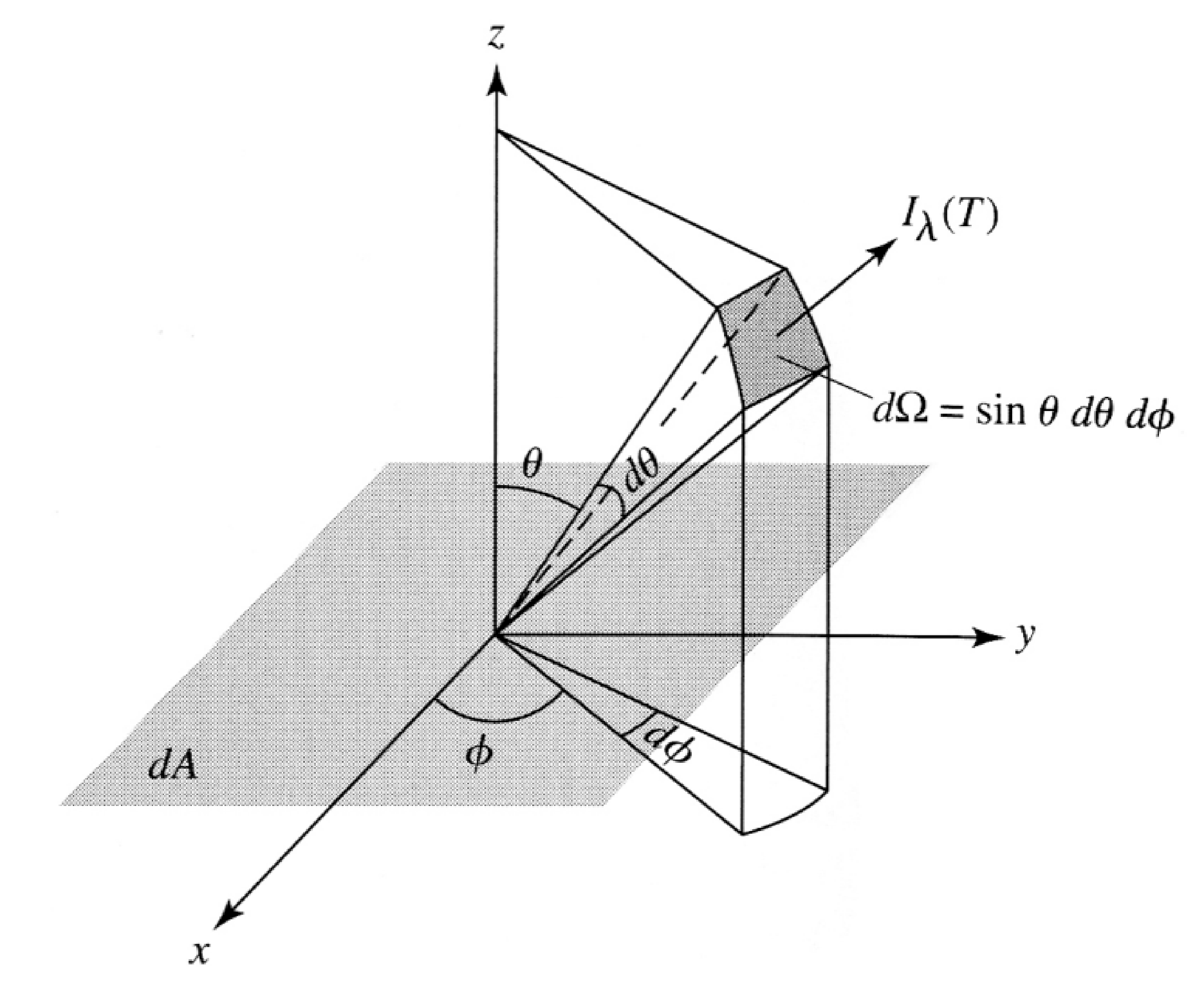
$$\vec{x}(s) = \vec{x}_0 + s\hat{n}$$

- Note: Intensity is constant in pure reflection and through lenses



Transport fundamentals: Moments

- The richness of angular information in the intensity makes it difficult to solve
- We can control this information by studying its moments by expanding the intensity into spherical harmonics
- We will inspect the zeroth, first, and second tensor moments of the field
- Disadvantage: Must specify an axis, breaking any possible rotational symmetries



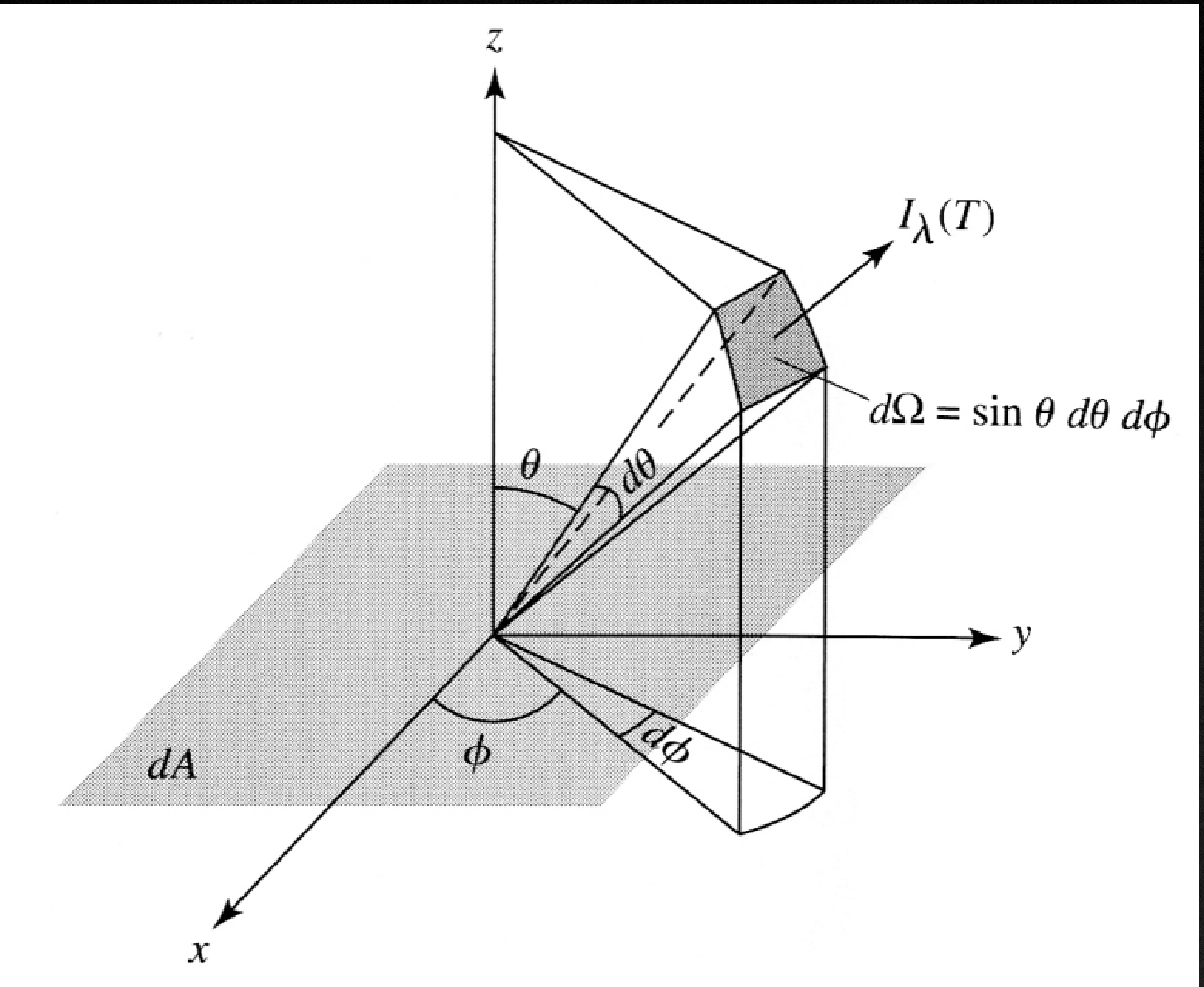
Transport fundamentals: Moments

- Zeroth moment (scalar): mean intensity averaged over angle

$$J_\nu = \frac{1}{4\pi}\oint I_\nu(\hat{n})d\Omega$$

- If the intensity is homogeneous and isotropic

$$J_\nu = I_\nu$$



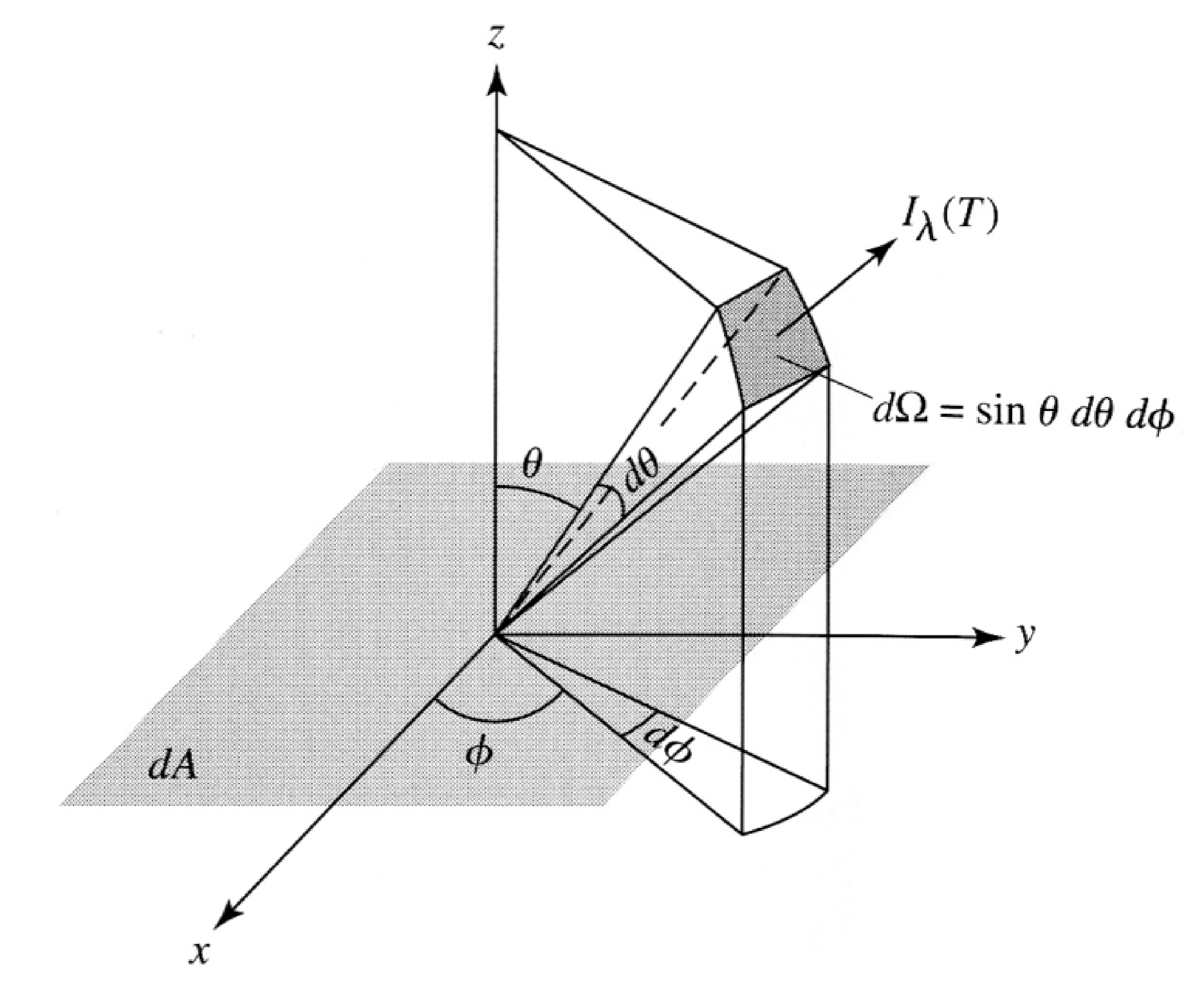
Transport fundamentals: Moments

- First moment (vector): average flow of energy, related to flux

$$\vec{H}_\nu = \frac{1}{4\pi}\oint I_\nu(\hat{n})\hat{n}\,d\Omega$$

- $\vec{F}_\nu = 4\pi\vec{H}_\nu$
- If the intensity is homogeneous and isotropic

$$\vec{H}_\nu = 0$$



Transport fundamentals: Moments

- Second moment (tensor): in radiation transport, this is related to the radiation pressure tensor

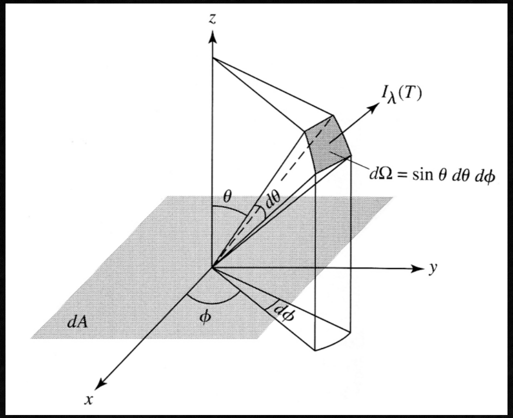
$$\mathcal{K}_\nu = \frac{1}{4\pi}\oint I_\nu(\hat{n})\hat{n}\hat{n}d\Omega$$

- Symmetric rank-2 tensor
- If the intensity is homogeneous and isotropic

$$\mathcal{K}_\nu = \frac{1}{3}\mathbb{I}J_\nu$$

- Here $\mathbb{I}$ is the unit rank-2 tensor

Transport fundamentals: Moments



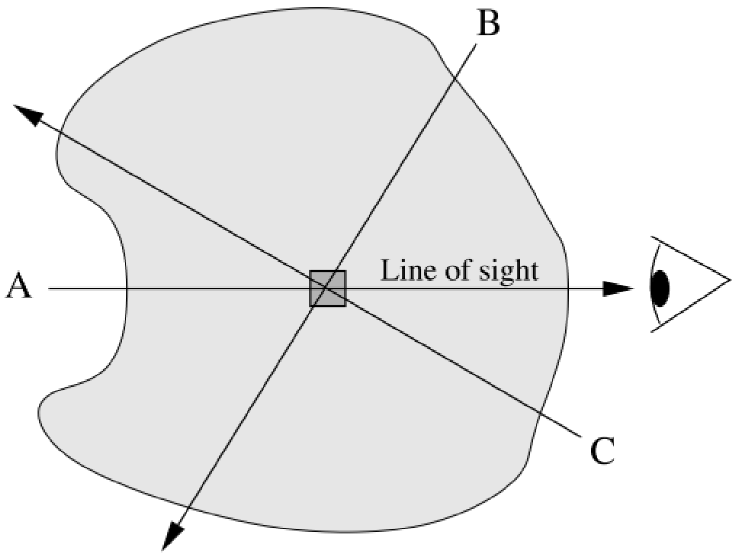
- We can write the moments more explicitly in terms of $\mu \equiv \cos\theta$

$$J_\nu = \frac{1}{4\pi}\oint I_\nu(\hat{n})d\Omega \quad\Rightarrow\quad J_\nu = \frac{1}{4\pi}\int_{-1}^{+1} d\mu \int_0^{2\pi} d\phi\, I_\nu(\mu,\phi)$$

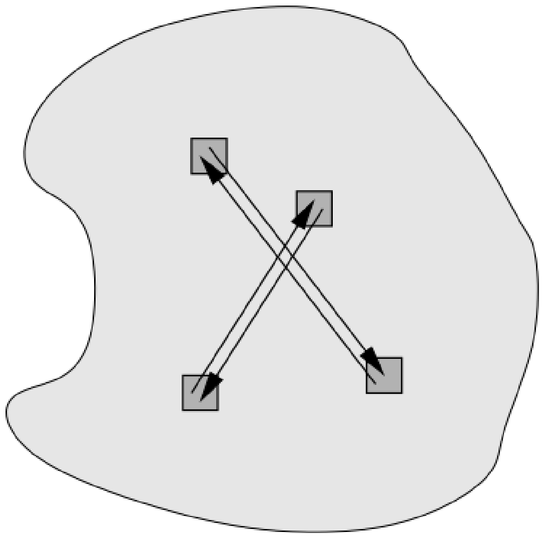
$$\vec{H}_\nu = \frac{1}{4\pi}\oint I_\nu(\hat{n})\hat{n}d\Omega \quad\Rightarrow\quad H_\nu^i = \frac{1}{4\pi}\int_{-1}^{+1} d\mu \int_0^{2\pi} d\phi\, I_\nu(\mu,\phi)\ n^i$$

$$\mathcal{K}_\nu = \frac{1}{4\pi}\oint I_\nu(\hat{n})\hat{n}\hat{n}d\Omega \quad\Rightarrow\quad K_\nu^{ij} = \frac{1}{4\pi}\int_{-1}^{+1} d\mu \int_0^{2\pi} d\phi\, I_\nu(\mu,\phi)\ n^i n^j$$

Ray coupling



Radiative cell coupling



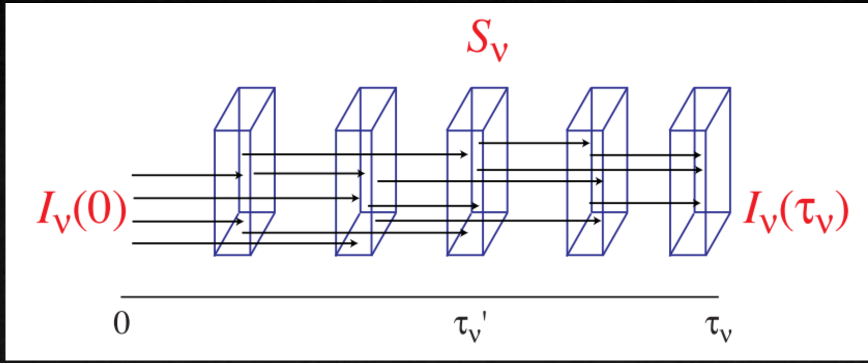
Why transport is difficult

- Transport is difficult because we don’t know the emissivity j_ν and/or extinction α_ν coefficients in advance
- However the radiation intensity $I_\nu(\vec{x}, \hat{n})$ can affect them and we need to calculate both
- This is a “chicken or egg” problem → to compute I_ν we need α_ν and j_ν, and vice versa.

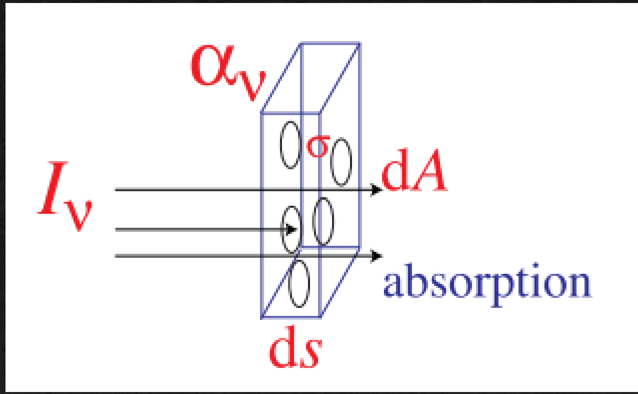
- Furthermore in the line of sight A (the problem of interest), radiation from directions B and C will affect the gas parcel where these directions intersect
- Lastly, each cell will affect each other

Radiative transfer equation (RTE)

- We will be now specializing toward the application of radiation, but the methods are general and can be applied to other transport equations
- Instead of a ray traveling in vacuum, consider a system that produces and absorbs photons



- Absorption: consider a species (e.g. atom, molecule) that absorbs a photon by excitation or ionization
- At some photon energy, the absorber has some cross-section σ

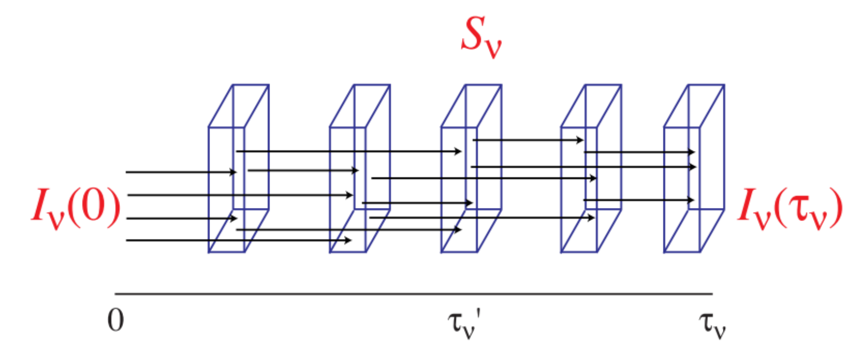


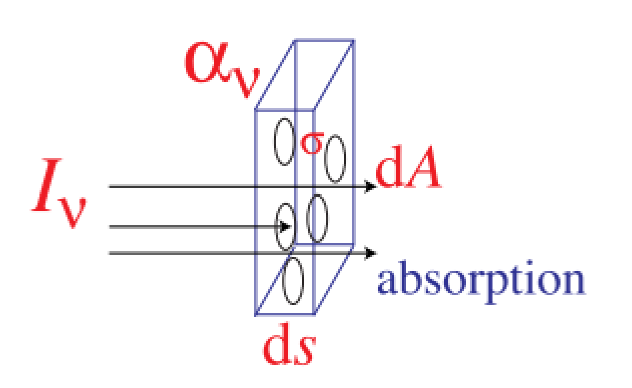
Radiative transfer equation (RTE)

- Given a number density n, the covering fraction

$$dA_{abs} = \sigma\, dN = \sigma n\, dV = \sigma n\, dA\, ds$$

- Absorption within this volume is random
- We can quantify the distance a photon travels before absorption as the mean free path l_{mfp}
  - Function of position and energy
- The extinction coefficient $\alpha_\nu = 1/l_{mfp}$ is used in the RTE





Radiative transfer equation (RTE)

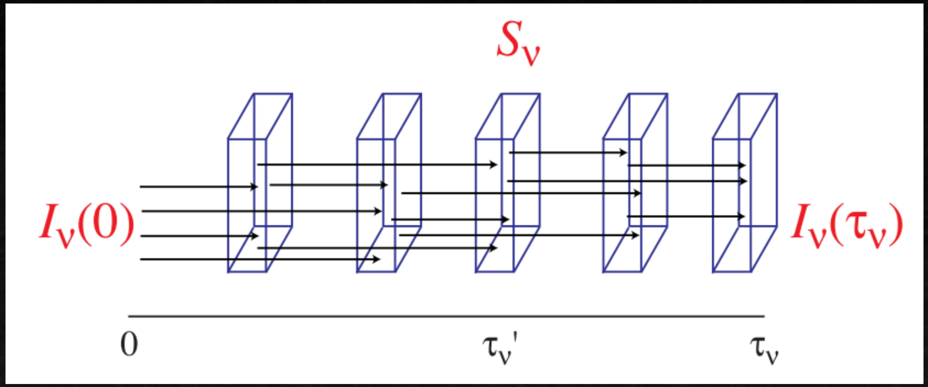
- The extinction coefficient $\alpha_\nu = 1/l_{mfp}$ is used in the RTE
- With absorption only, the intensity along a ray behaves as

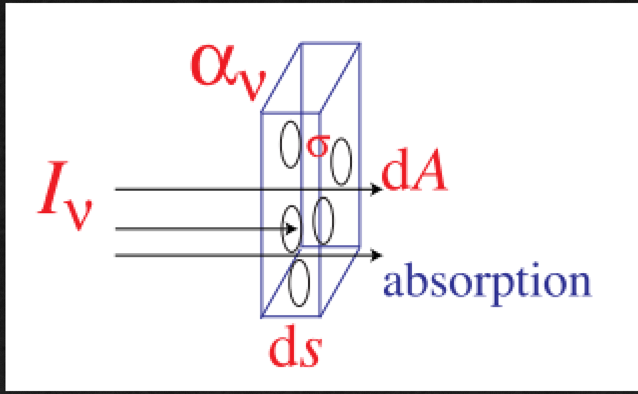
$$\frac{dI_\nu(\hat{n}, s)}{ds} = -\alpha_\nu(s) I_\nu(\hat{n}, s)$$

- That has the integral form

$$I_\nu(\hat{n}, s_1) = I_\nu(\hat{n}, s_0) \exp[-\tau_\nu(s_0, s_1)]$$

- Here $\tau_\nu = \int_{s_0}^{s_1} \alpha_\nu ds$ is called the optical depth

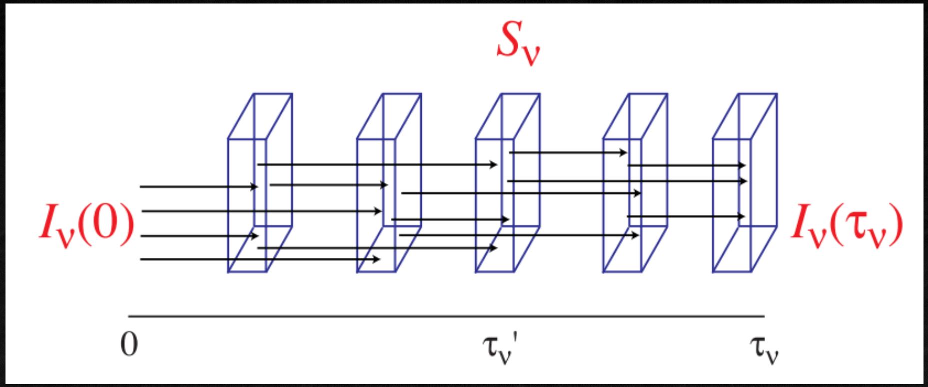




Radiative transfer equation (RTE)

- We can now introduce emission of photons into the RTE through the emissivity $j_\nu(s)$

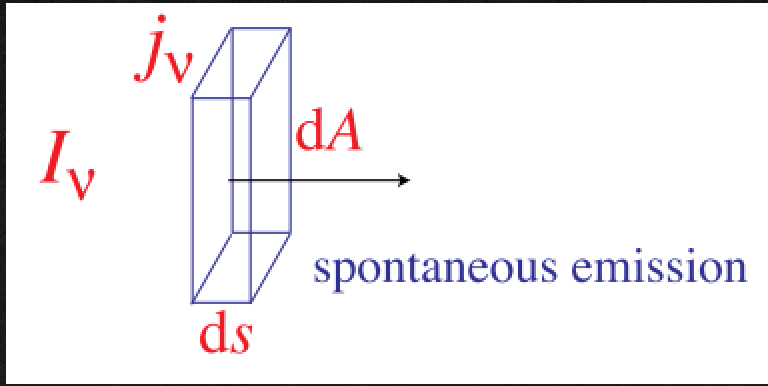
$$\frac{dI_\nu(\hat{n},s)}{ds} = j_\nu(s) - \alpha_\nu(s) I_\nu(\hat{n},s)$$



- We can also define the source function $S_\nu \equiv j_\nu/\alpha_\nu$ so that

$$\frac{dI_\nu(\hat{n},s)}{ds} = \alpha_\nu(s)[S_\nu(s) - I_\nu(\hat{n},s)]$$

- In local thermal equilibrium, the source function is the Planck function

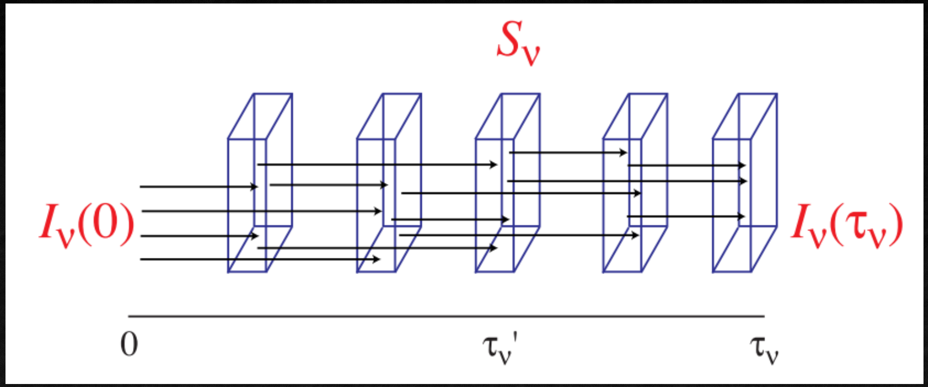


Radiative transfer equation (RTE)

- Here the integral form is

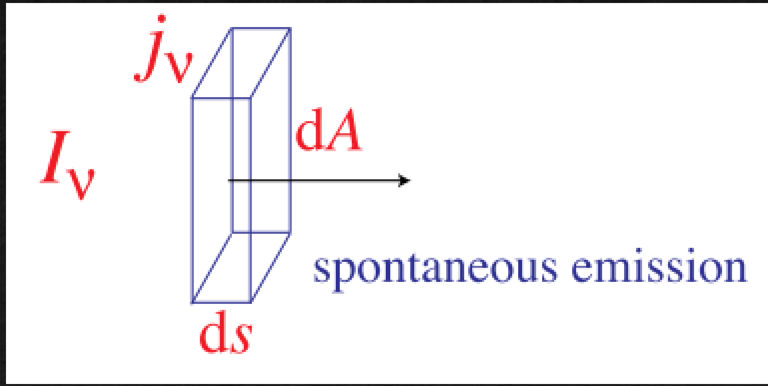
$$I_\nu(\hat{n}, s_1) = I_\nu(\hat{n}, s_0)\exp[-\tau_\nu(s_0, s_1)] +$$

$$\int_{s_0}^{s_1} j_\nu(s)\exp[-\tau_\nu(s, s_1)]ds$$



- The general 3D form of the RTE is

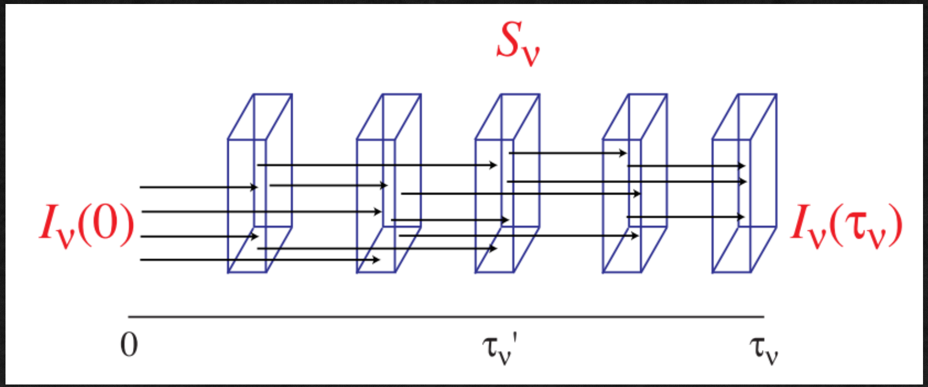
$$\hat{n} \cdot \nabla I_\nu(\vec{x}, \hat{n}) = j_\nu(\vec{x}) - \alpha_\nu(\vec{x}) I_\nu(\vec{x}, \hat{n})$$

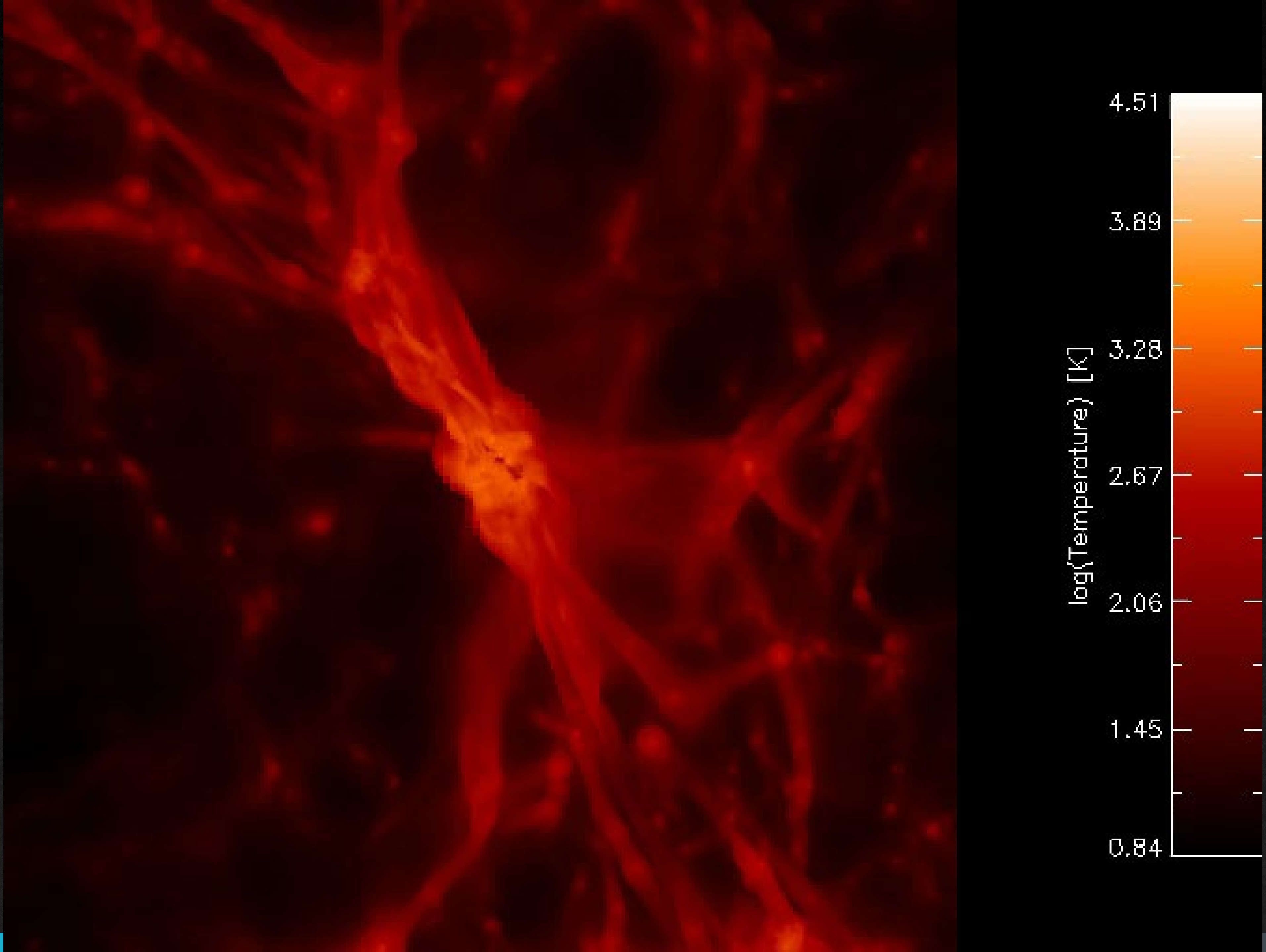


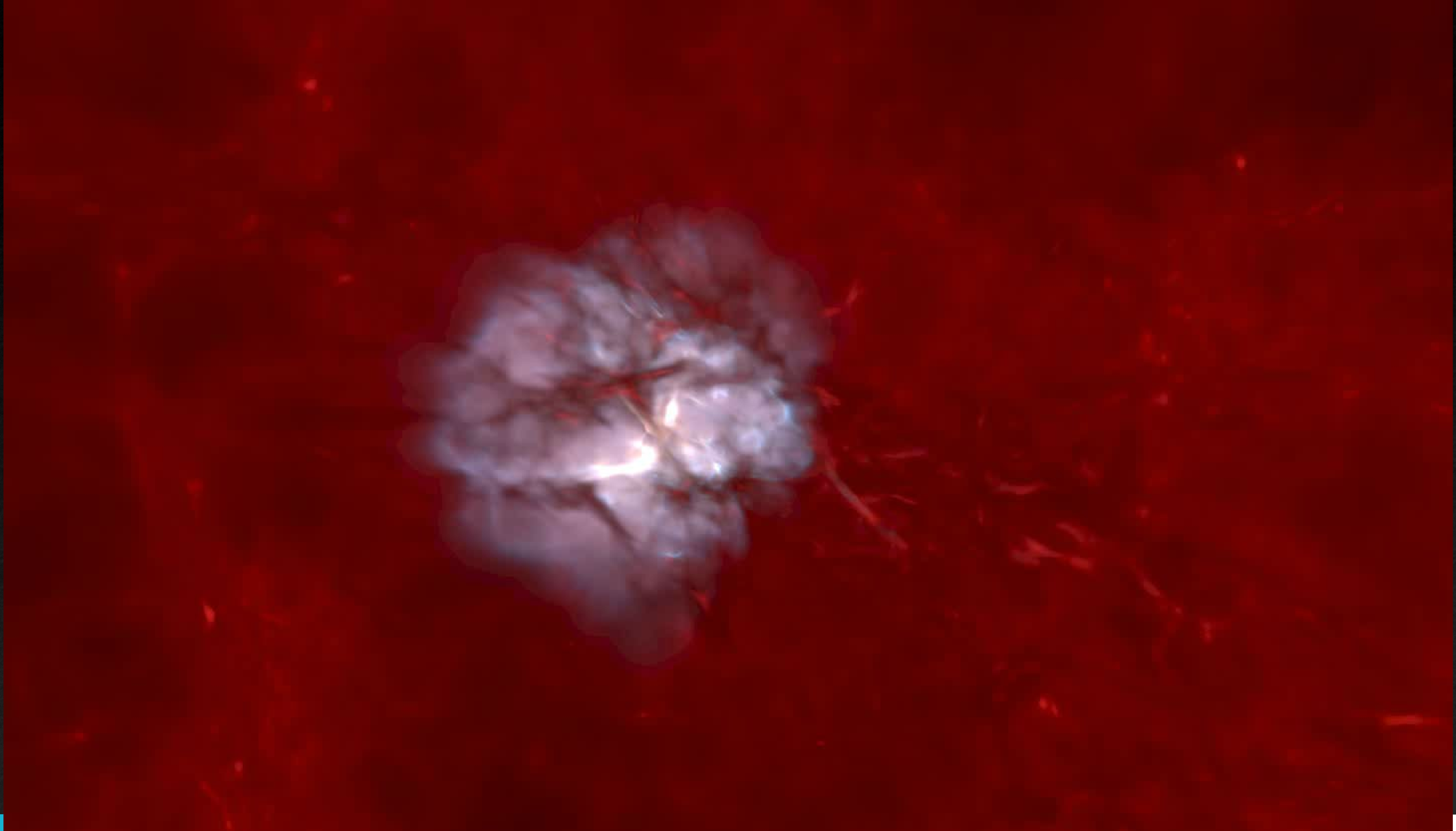
Radiative transfer equation (RTE)

- So far, we've been considering the time-independent case
- If the system is evolving or we want to forward model it, the RTE becomes

$$\frac{1}{c}\frac{\partial I_\nu(\hat{n},s,t)}{\partial t} + \frac{\partial I_\nu(\hat{n},s,t)}{\partial s} = j_\nu(s) - \alpha_\nu(s) I_\nu(\hat{n},s,t)$$

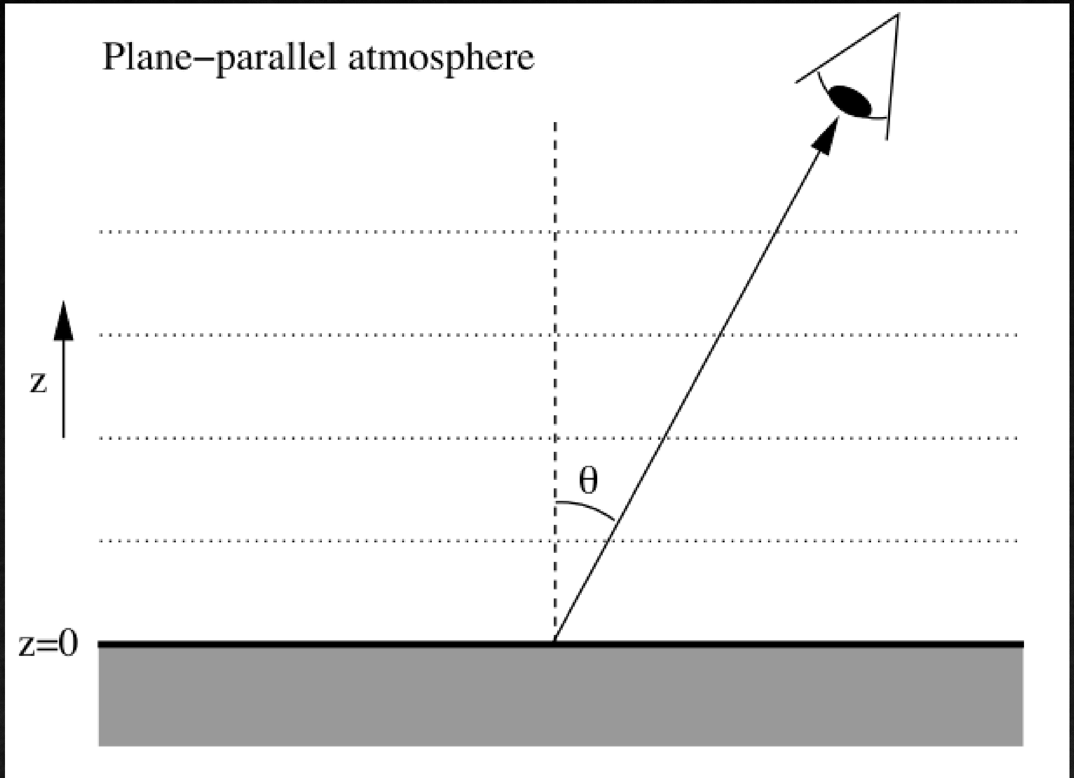



4.51
3.89
3.28
2.67
2.06
1.45
0.84
log(Temperature) [K]



1D plane-parallel radiative transfer

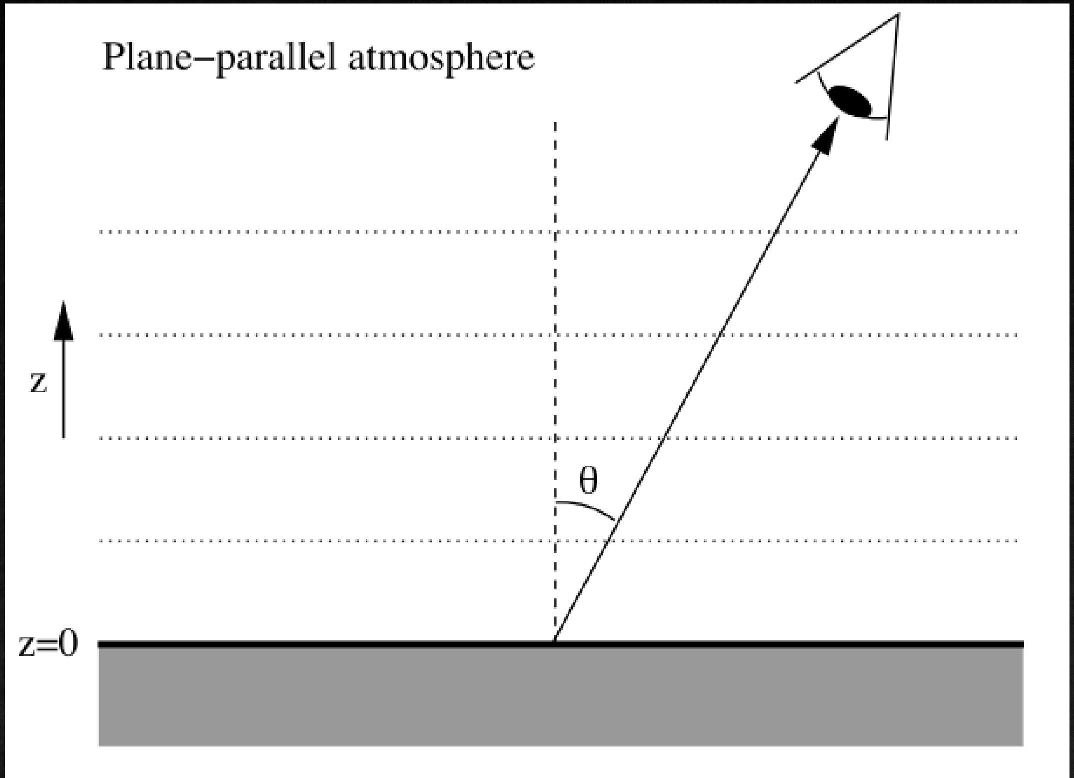
- In some systems, we can identify symmetries to reduce the dimensionality
- In a plane-parallel system, the only spatial dependence is in the z-direction
- This symmetric also has rotational symmetry, dropping the dependence on ϕ
- Leaves only a 3D problem: height z, angle coordinate $\mu \equiv \cos\theta$, frequency ν



1D plane-parallel radiative transfer

- The $\partial/\partial x$ and $\partial/\partial y$ operators yield zeros, and d/ds becomes $\mu d/dz$
- Thus the RTE in a plane-parallel problem transforms into

$$\mu \frac{dI_\nu(z,\mu)}{dz} = \alpha_\mu(z)[S_\nu(z) - I_\nu(z,\mu)]$$



1D plane-parallel radiative transfer

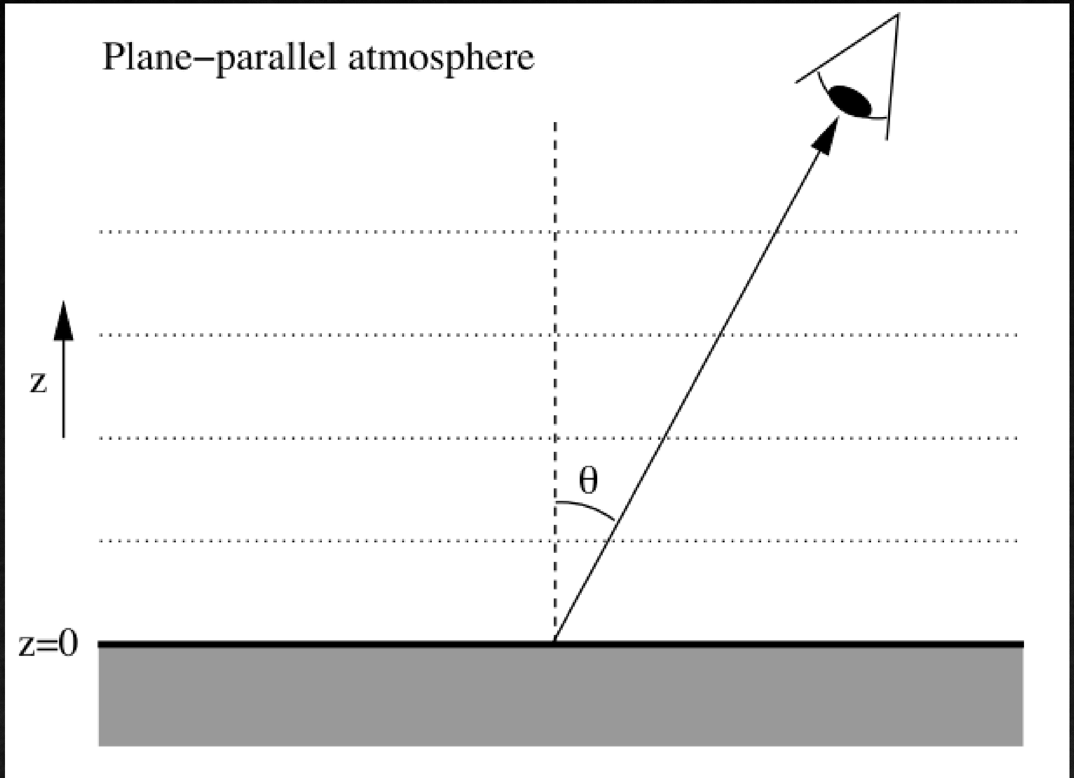
$$\mu \frac{dI_\nu(z,\mu)}{dz} = \alpha_\mu(z)[S_\nu(z) - I_\nu(z,\mu)]$$

- Moments (all scalars because we are only interested in the z-component)

$$J_\nu = \frac{1}{2}\int_{-1}^{+1} I_\nu(\mu) d\mu$$

$$H_\nu = \frac{1}{2}\int_{-1}^{+1} I_\nu(\mu)\, \mu\, d\mu$$

$$K_\nu = \frac{1}{2}\int_{-1}^{+1} I_\nu(\mu)\, \mu^2\, d\mu$$

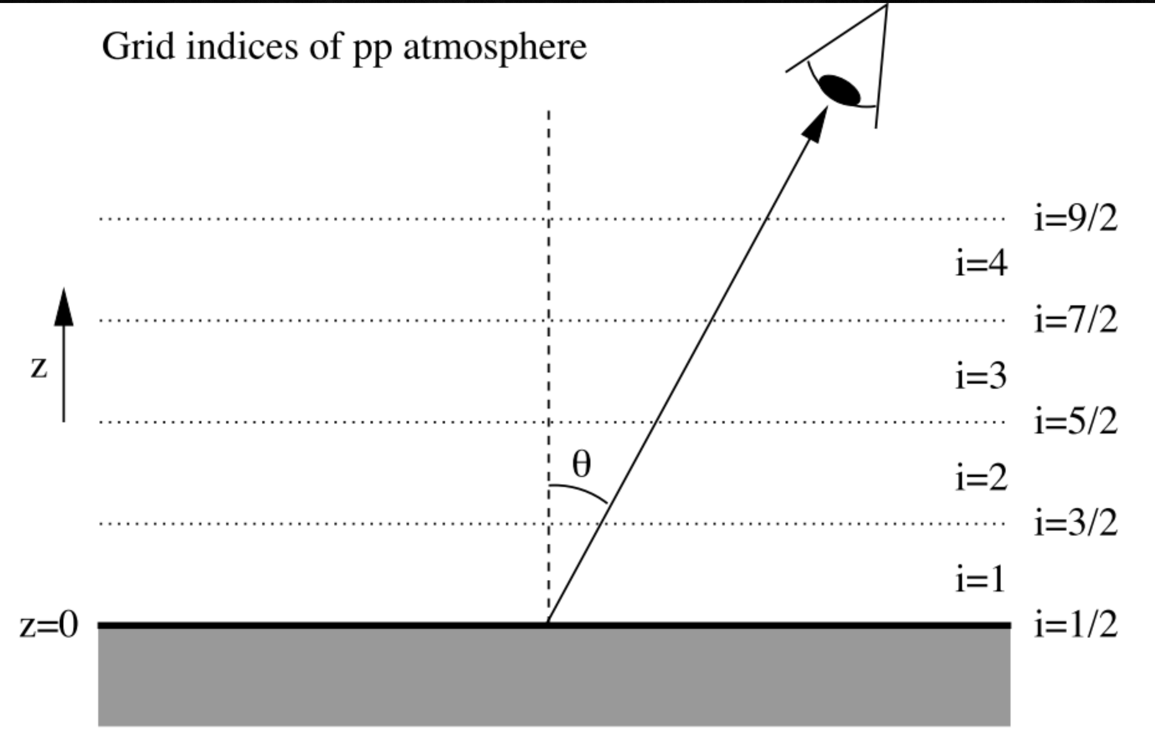


1D plane-parallel radiative transfer: numerical

- We want to integrate

$$\frac{dI}{ds} = j - \alpha I \equiv \alpha(S - I)$$

- We will omit $\vec{x}, \hat{n}, \nu$ for convenience.
- Let's look at the Olson & Kunasz (1987) method
  - Assume a functional form of j(z) and $\alpha(z)$ between the cell boundaries
  - Solve the RTE exactly between the boundaries



1D plane-parallel radiative transfer: numerical

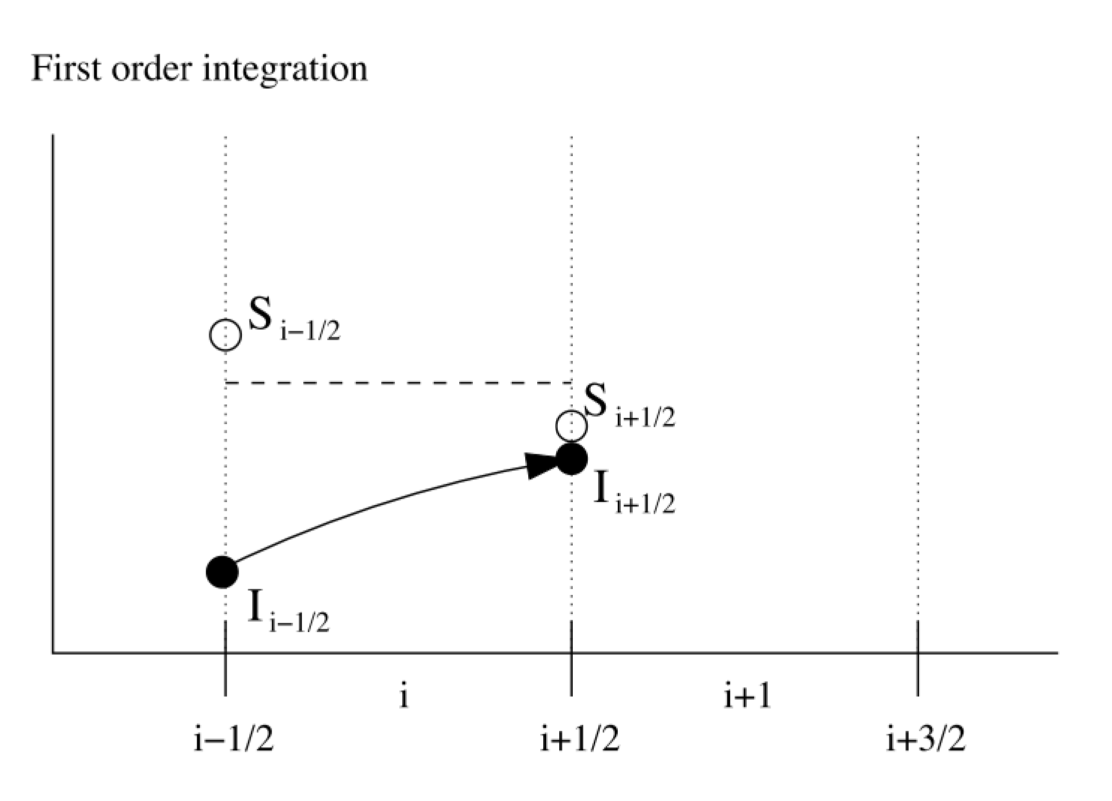
- First order integration: assume constant emissivity j and extinction α within the cell
- For each cell i, calculate an optical depth

$$\Delta\tau_i = \left(s_{i+1/2} - s_{i-1/2}\right)\alpha_i$$

- Using the source function $S_i = j_i/\alpha_i$, the intensity at the next cell boundary is

$$I_{i+1/2} = e^{-\Delta\tau_i} I_{i-1/2} + \left(1 - e^{-\Delta\tau_i}\right)S_i$$

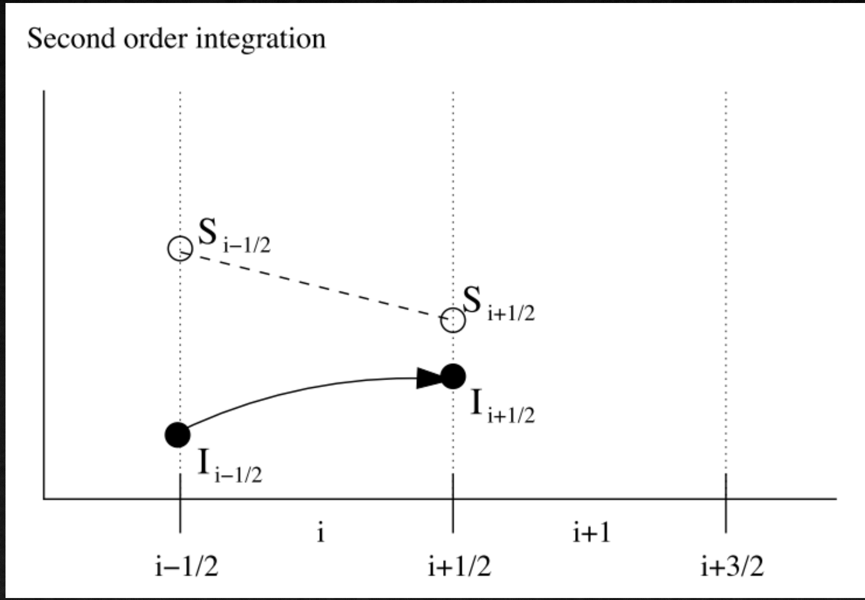
- Repeat for all angles μ



1D plane-parallel radiative transfer: numerical

- Second order integration: assume linear emissivity j and extinction α within the cell
- The optical depth remains the same

$$\Delta\tau_i = \left(s_{i+1/2} - s_{i-1/2}\right)\alpha_i$$

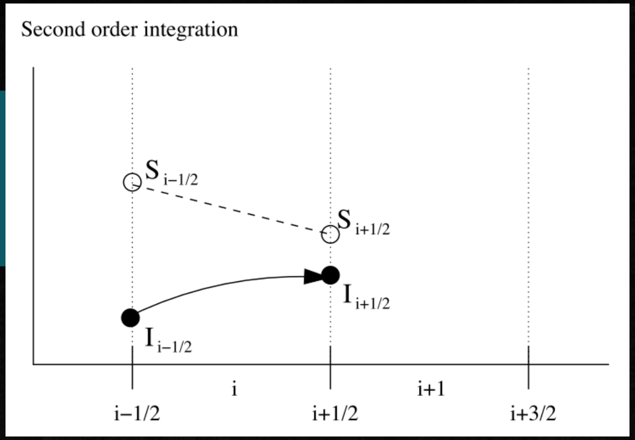


- The exact solution of the RTE across the cell is

$$I_{i+1/2} = e^{-\Delta\tau_i}\, I_{i-1/2} + Q_i$$

$$Q_i = \left[\frac{1-(1+\Delta\tau_i)e^{-\Delta\tau_i}}{\Delta\tau_i}\right] S_{i-1/2} + \left[\frac{\Delta\tau_i - 1 + e^{-\Delta\tau_i}}{\Delta\tau_i}\right] S_{i+1/2}$$

1D plane-parallel radiative transfer: numerical



$$I_{i+1/2} = e^{-\Delta\tau_i} I_{i-1/2} + Q_i$$

$$Q_i = \left[\frac{1-(1+\Delta\tau_i)e^{-\Delta\tau_i}}{\Delta\tau_i}\right] S_{i-1/2} + \left[\frac{\Delta\tau_i - 1 + e^{-\Delta\tau_i}}{\Delta\tau_i}\right] S_{i+1/2}$$

- When $\Delta\tau_i$ is small, we need to use the limit instead of a direct evaluation to avoid divisions by zero, where

$$\lim_{\Delta\tau_i \to 0} Q_i = \frac{1}{2}\Delta\tau_i\left(S_{i-1/2} + S_{i+1/2}\right)$$

Monte Carlo radiative transfer

- Follow many (thousands, millions, billions) rays, solving the RTE along each path, until we have a good statistical sample of the radiation field

- Easy to understand because they simulate the motion of photons
- Easy to implement complicated microphysics in a bulk manner
- Each ray has some direction $\hat{n}$ and current position $\vec{x}$
- Can consider the head of the ray as a “photon packet” traveling through the domain

- Let’s first look at a pure scattering problem, i.e. $\epsilon_\nu = 0$

MCRT: Finding the next scattering event

- Scattering is not a deterministic process, but it follows a Poisson distribution
- Generate a random number to find the optical depth τ of the next scattering event, which has a PDF of

$$p(\tau) = e^{-\tau}$$

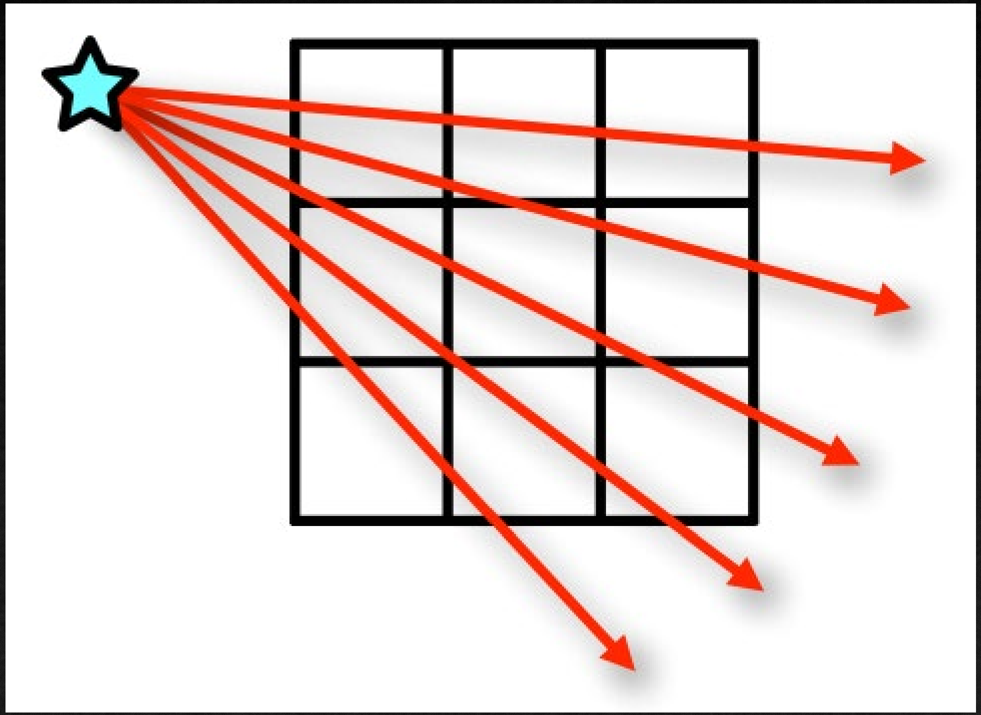
- Which can be achieved by drawing a uniform random number $\xi \in (0,1]$ that corresponds to a random optical depth

$$\tau = -\ln \xi$$

MCRT: Finding the next scattering event

- Ray trace through the domain points, solving the RTE in each cell, until we reach the previously determined τ
- Each cell will have some optical depth $\Delta\tau$

- Also, a ray may exit the domain without being scattered, in which case we delete the ray and proceed to the next ray



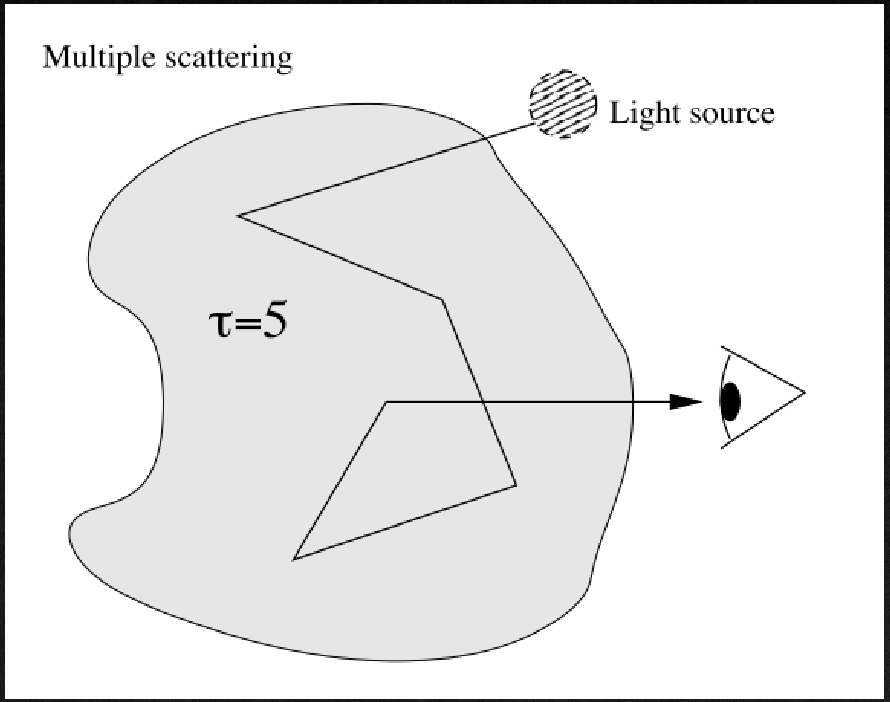
MCRT: drawing a random scattering direction

- When we reach the cell where the scattering event occurs, a new direction much be drawn

- In the isotropic scattering case, we want the directions to be uniformly distributed around the unit sphere, giving

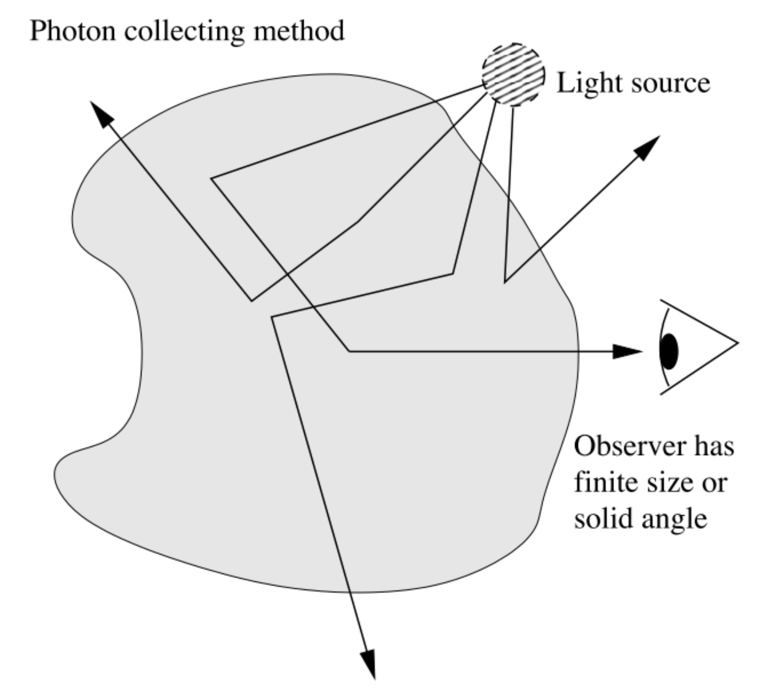
$$\theta = \cos^{-1}(2\xi_1 - 1)\,, \qquad \phi = 2\pi\xi_2$$

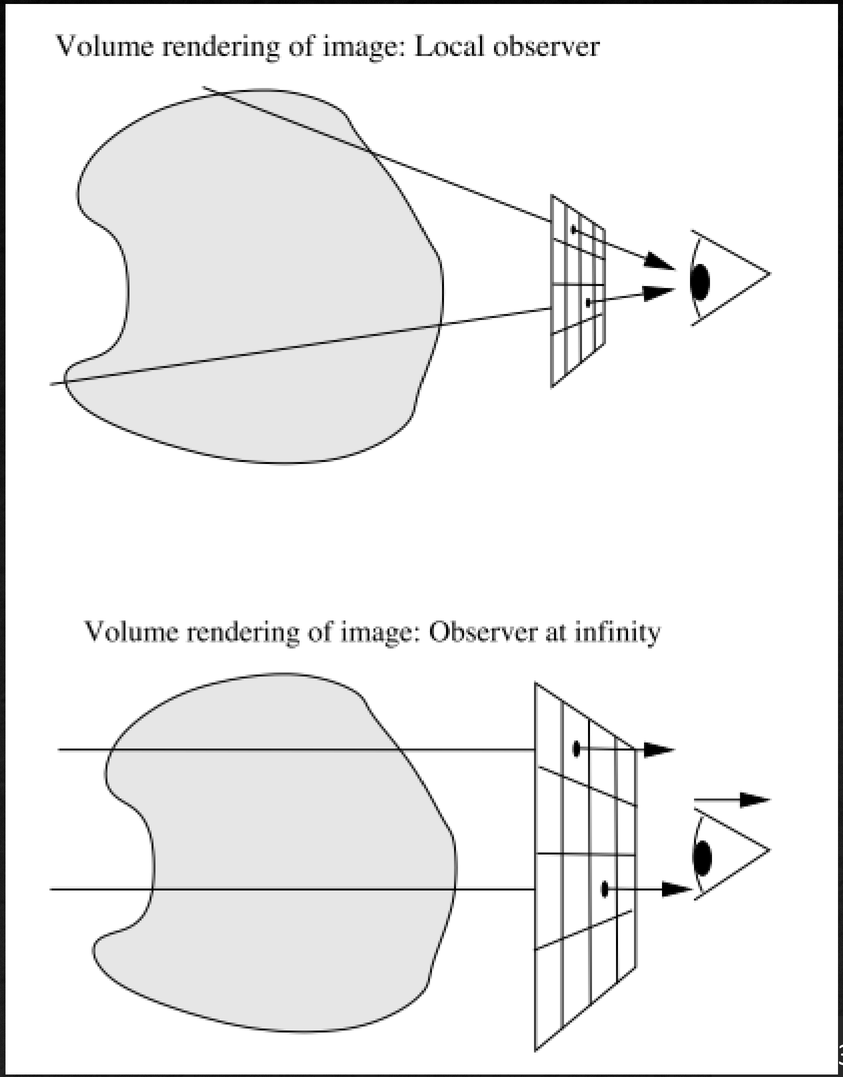
where ξ_i are uniform random numbers.



MCRT: synthetic images

- Different methods to create images from scattered light
- In all cases, we solve the RTE along those rays
- Choose perspective depending on problem



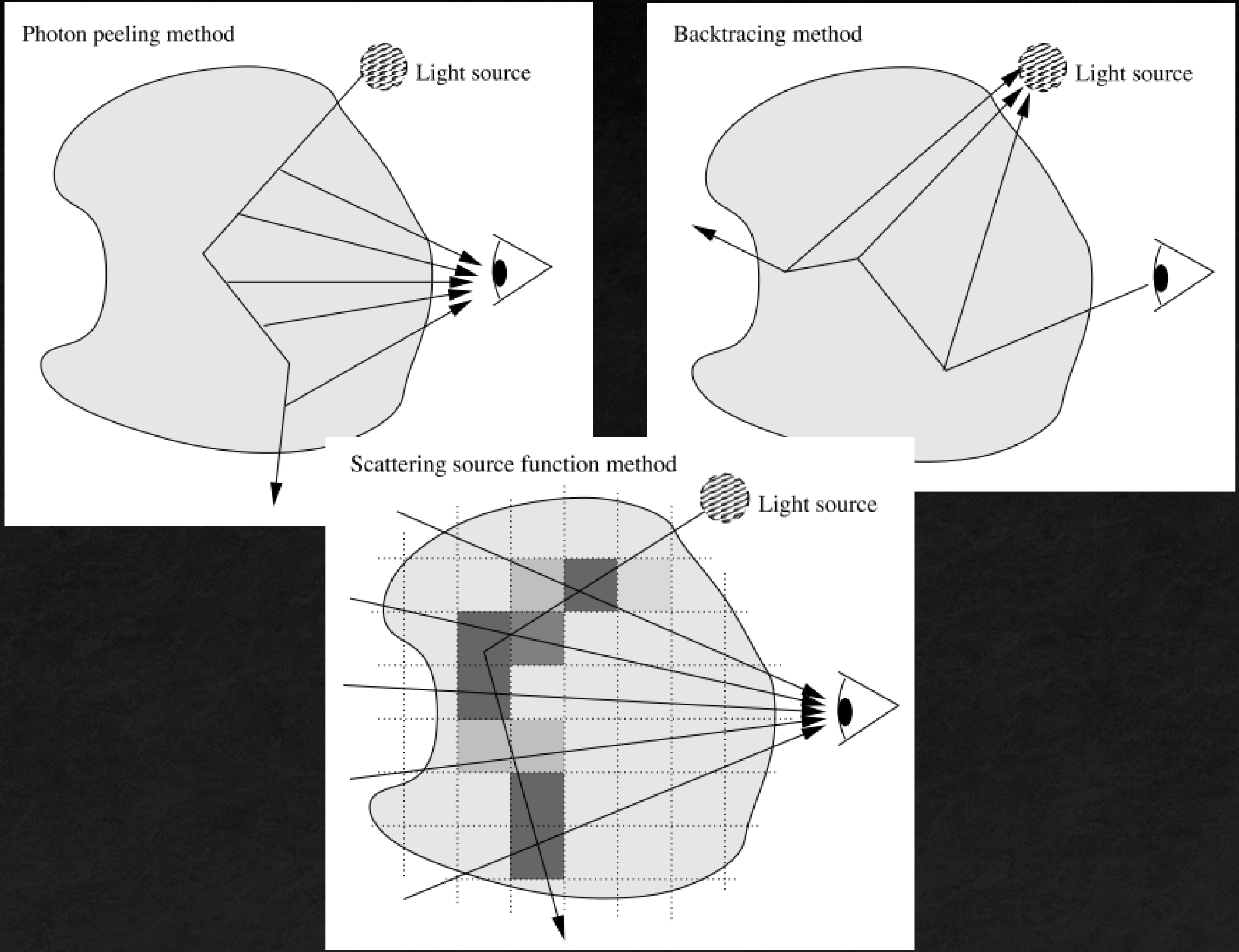


MCRT: synthetic images

- Three popular methods

1. Photon peeling
2. Backtracing
3. Scattering source function

- Usually need $O(10^6)$ photons to reduce MC noise



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