복사전달 특강

Special Topics in Radiative Transfer

Lecture 9

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Based on: Chapter 7 of Noebauer & Sim (Living Reviews in Computational Astrophysics)

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Chapter 7: Thermal and Line Emission in MCRT

Overview of approaches to emission in MCRT

- Absorption/scattering treatment in MCRT is relatively simple, standard and well-established.
- However, emission handling methods are varied, complex, and site of ongoing developments.

Here, we focus: emissivity **within** the computational domain (not boundary injection, cf. Sect. 5.3)

7.1 Known Emissivity

- The easiest case is the emissivity given externally.
- Direct sampling — no self-consistency
- Example: non-radiative heating and ionization

7.2 Radiative Equilibrium (RE)

- Emissivity is not known a prior, but set by radiation field itself.
- Local balance: absorption = emission
- Emissivity cannot be known without RT simulation.

7.3 Radiative Equilibrium by Iteration

- Iterative RT simulations, In each iteration, the current best estimate of the conditions (T, ionization state, level populations) in the medium is adopted to make an improved estimate for those conditions in the next cycle.
- The non-local character of RT problems can lead to significant convergence issues at high optical depth.
- Energy conservation is only achieved asymptotic.

7.4 On-the-fly RE (Indivisible Packets)

- It is simple to rigorously enforce the conservation of energy required by RE via an **indivisible energy packet**.
- MC quanta never destroyed or degraded. All interactions (including pure absorption) between MC packets and the medium become effective scatterings controlled by rules, which depend on the physical processes being simulated.
- Strict RE at every packet event.

7.5 Beyond Radiative Equilibrium

External non-radiative heating (H_{E}) and expansion cooling (C_{E}) added as source/sink terms

Applied in: stellar outflows, SNe codes, accretion disc winds

7.1 Known Emissivity

Simplest case: emissivity given without prior knowledge of the radiation field

- Applies when emissivity is externally known or easily estimated independently
- Example: non-equilibrium plasma heated/ionised by non-radiative processes

Procedure

1. Sample emissivity using standard sampling techniques (Sect. 4.2)
2. Create packets representing the emission process:
   - Photon frequency ν — sampled from the emissivity spectrum
   - Weight / energy — set by the emissivity normalisation
   - Propagation direction — sampled from the angular distribution
3. Inject alongside any packets from external boundary conditions
4. Follow their subsequent propagation in the same way

Time-dependent Extension

In time-dependent simulations, emission packets are injected gradually over the time step.
The injection time t_{inj} is an additional property to be sampled (uniformly over Δt).

Key advantage: no iteration required — emissivity is decoupled from the radiation field.
Simply add these source packets alongside any other packet populations and propagate.

7.2 Radiative Equilibrium (RE)

When the emissivity is determined by the radiation field itself

What is Radiative Equilibrium?

At every point in the medium there is local balance between absorption and emission of radiation:

Rate of absorption = Rate of emission

Emissivity is effectively determined by the radiation field (near-equilibrium) and cannot be anticipated independently of a RT simulation.

Astrophysical Applications

- Stellar and disk atmospheres
- Hot-star winds
- Type Ia Supernovae (SN Ia)
- Cataclysmic variable accretion disc winds
- Active galactic nuclei winds

→ RE is a good approximation for many key RT problems in astrophysics

Challenge: Emissivity depends on the radiation field, but the radiation field depends on the emissivity → must be solved self-consistently.

- Two strategies:
- Sect. 7.3 — RE by iteration: run RT repeatedly until convergence
- Sect. 7.4 — On-the-fly: use indivisible energy packets so RE is enforced at every event

7.3 Radiative Equilibrium in MCRT by Iteration

Solving RE via a sequence of radiative transfer simulations

Iterative Scheme

1. Start with initial estimate of medium conditions (T, ionisation state, level populations…)
2. Calculate emissivity from current conditions
3. Run MCRT simulation → extract updated radiation field estimators
4. Use RT outcomes to obtain improved estimate of conditions
5. Repeat steps 2–4 until convergence

When It Works

- Applicable to photon-packet and energy-packet schemes
- Used for part of emissivity, e.g. radiative cooling (Long & Knigge 2002)
- Works when optical depth is not too severe

Convergence Problems

- Non-local RT character can lead to significant convergence problems (→ slow convergence)
- This issue is especially sever at high optical depth.
- Energy conservation is only achieved asymptotic.
- Over/under-estimated emissivities create spurious energy sources and sinks

Historical Perspective

Well-known from stellar atmospheres (Hubeny & Mihalas 2014): non-local RT inhibits convergence at high τ.

Motivation for Sect. 7.4: enforce RE exactly at every packet event without any iteration.

7.4 On-the-fly RE via Indivisible Energy Packets

The key idea: enforce energy conservation as a Monte Carlo rule

- Developed by Lucy (Abbott & Lucy 1985; Lucy 1999a, 2005)

Key Principle: RE requires local balance between absorption and emission of energy.
In an energy-packet discretization, MC quanta already represent bundles of radiative energy.

→ MC quanta are NEVER destroyed or degraded in weight during the simulation.
→ ALL interactions — even those representing pure absorption — become effective scatterings.

Indivisible Packet Principle

- Each MC packet carries fixed energy ε (invariant).
- Absorption event → packet immediately re-emitted (in situ)
- Packet energy conserved at every interaction
- Strict RE enforced — no spurious sources/sinks

Contrast with Sect. 7.3: RE enforced locally at each event, not asymptotically at convergence

Rules for Effective Scattering

The rules for how a packet's properties (frequency, direction) change depend on the physical process:

- Statistical equilibrium → traffic flow rules (Sect. 7.4.1–7.4.4)
- Thermal equilibrium (TE) → k-packet rules (Sect. 7.4.5)

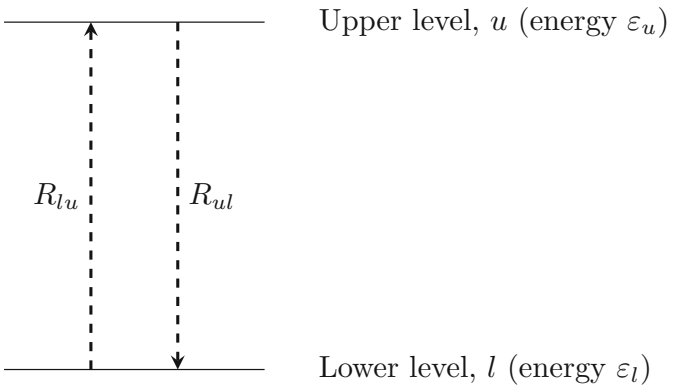
Formulated generally by Lucy (2002, 2003)

7.4.1 Example: Effective Resonant Scattering in a Two-level Atom

Simplest illustration of the indivisible packet RE principle (Lucy 1999a)

Assumptions:

- Spectral line absorption in a two-level atom (see Fig. 5 →)
- Radiation dominates excitation/de-excitation; isotropic emission
- Stimulated emission treated as negative absorption



Line Emissivity

$$\eta_{ul} = \frac{h\nu}{4\pi}\psi_{ul}(\nu)R_{ul}$$

$\psi_{ul}(\nu)$ = emission profile function (normalized): $\int \psi_{ul}(\nu)d\nu = 1$

Transition Rate

$$R_{ul} = n_u A_{ul}$$

n_u = upper-level population, A_{ul} = Einstein-A coefficient

The Problem

Need n_u to evaluate n_{ul}, but n_u is unknown until after the RT simulation.
→ Statistical equilibrium provides the resolution (see next slide).

7.4.1 MCRT Rule for Two-level Atom

Statistical equilibrium as a traffic flow condition

Provided that **statistical equilibrium ($R_{ul} = R_{lu}$)** applies, this statement can be used to replace a direct evaluation of the emissivity.

Rate of absorption from the radiation field = Rate of emission into the radiation field

MCRT Implementation — Traffic Flow Rule

Whenever an MC energy packet is absorbed by the spectral line → it is immediately (in situ) re-radiated by the same line.

- Absorption of packet ←→ realization of R_{lu} (inflow term)
- Re-emission of packet ←→ realization of R_{ul} (outflow term)

New direction and frequency sampled from $\psi_{ul}(\nu)$; packet energy ε conserved.

The statistical equilibrium equation is thus embedded as a processing rule — no knowledge of n_u needed in calculating R_{ul}.

Key Features

- Leading n_u dependence cancels via normalization
- Strict energy conservation at every event
- MC packets never destroyed
- Simple and fast to implement

- Used in: Abbott & Lucy 1985; Long & Knigge 2002; Kusterer et al. 2014

Physical Justification & Limitations

- Well justified for strong UV metal lines:
  C IV 1550 Å, N V 1242 Å in stellar winds

- Limitation of the two-level approximation:
  — not realistic when fluorescence or thermal reprocessing is important

→ Extended in next slides (Sects. 7.4.2–7.4.4)

7.4.2 Fluorescence & Thermal Emissivity via Redistribution Parameters

Extending indivisible packets to handle flux redistribution

- Redistribution parameter Λ is introduced (Baron et al. 1996; Pinto & Eastman 2000a,b; Kasen et al. 2006)

At each packet interaction: draw random number ξ ∈ [0, 1] and compare to Λ:

ξ > Λ → Coherent scattering: new direction assigned; CMF (co-moving frame) frequency conserved
(as in electron scattering or resonance line scattering)

ξ ≤ Λ → Incoherent (effective) scattering: new direction + new frequency

- new frequency must be drawn from a normalized emissivity distribution, e.g. LTE thermal: $\chi_\nu B_\nu$
- fully redistributive

Setting Λ

- Global constant, or per-interaction type
- For line scattering:
  It can be estimated by comparing collisional vs. radiative de-excitation rates (similar to Long & Knigge 2002)

- Λ → 1: nearly coherent scattering.
  This type of approach is similar to the case of known emissivity.
  However, the notable difference is that here the absolute normalization of the emissivity is not used, and strict RE is still enforced in the radiation/matter interactions.

Demonstrated Success for SN Ia

Baron et al. 1996; Pinto & Eastman 2000a,b; Kasen et al. 2006; Magee et al. 2018:

Thermal redistribution (a simple Λ) captures flux redistribution in SN Ia well and agrees with more detailed treatments.

7.4.3 Multi-level Atoms: Downbranching Scheme

Extending traffic flow rules to handle fluorescence and cascades (Lucy 1999b)

- Problem: fluorescence couples multiple spectral lines → cannot be described by a single redistribution emissivity

Downbranching Scheme — Lucy (1999b)

When an energy packet is absorbed via transition to upper level u,

re-emit in transition $u \rightarrow l$ with probability proportional to the energy flow rate: $$q_{u \rightarrow l} = \frac{R_{ul}\varepsilon_{ul}}{\sum_{k<u} R_{uk}\varepsilon_{uk}}$$

Use energy flow rates (not pure transition rates) because packets carry fixed energy.

Only downward transitions ($u \rightarrow l$, $l < u$) are considered.

Strengths

- Large improvement over resonance scattering for SN spectra (Lucy 1999b; Mazzali 2000)
- Performs extremely well even compared to full macro atom (Kerzendorf & Sim 2014)
- Computationally efficient

Limitations

- Only downward transitions allowed.
- Cannot handle inverse fluorescence (1→2, 2→3 absorption followed by 3→1 emission)
- Formally derived assuming downward rates dominate and $\varepsilon_u \gg \varepsilon_l$

Motivation for Macro Atom

A complete solution must include ALL transitions (upward and downward).
→ Full macro atom method (Lucy 2002, 2003)

7.4.3 The Macro Atom Method

General framework for multi-level atoms in radiative and statistical equilibrium

Central Concept — Lucy (2002, 2003)

- In the macro atom method, all excited levels of the matter is viewed as energy pools.
- Energy flows in/out of each pool via the "complete" set of radiative and collisional transitions and the equilibrium condition (i.e., energy associated with each pool is stationary) is satisfied by imposing a traffic flow set of rules to process interactions for each possible energy level.

- Sophistication compared with downbranching scheme is that **we include not only energy flow to and from the radiation field, but also between the energy pools associated with the levels of atoms/ions/molecules** (internal radiationless transitions)

(1) radiation field ↔ matter internal states, and (2) matter internal state ↔ matter internal state.

Three Types of Events

Activation:
absorbed packet → energy enters excitation pool
Deactivation:
emitted packet → energy leaves excitation pool

Internal transition: radiationless transfer between pools

Advantages over Downbranching

- Handles ALL transitions (upward + downward)
- Captures inverse fluorescence naturally

- Two-level and downbranching are special limits (macro atom with ε_1 = 0 or suppressed internals)

Key Result (Lucy 2002)

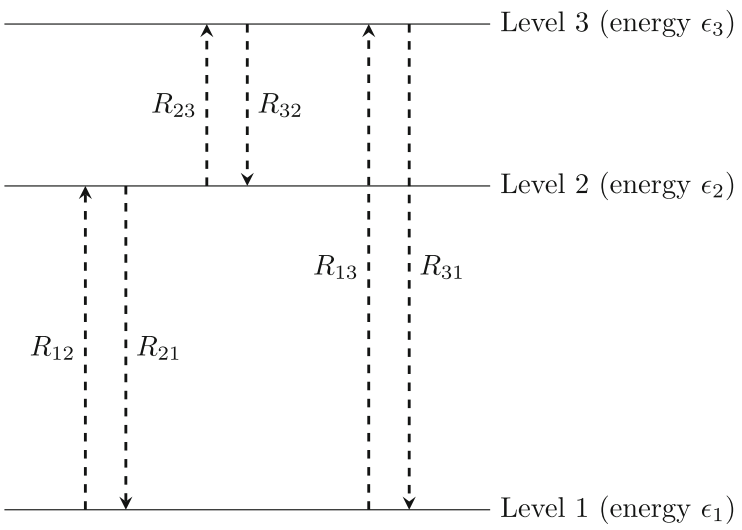
Level populations n_i cancel from transition probabilities → macro atom works without converged level populations.
Demonstrated for Fe II (Lucy 2002, Fig. 5).

7.4.4 Macro Atom for a Three-level Atom

Deriving macro atom rules from statistical equilibrium (bound-bound only, radiation-dominated)

For simplicity, assume:

- Bound-bound only; radiation dominates all rates; isotropic emission; no collisions
- Goal:
  To formulate rules for packets absorbed in lines ν_{12}, ν_{13}, ν_{23}



Statistical Equilibrium Equations

Rates into level = rates out of level for each level:

Level 1: $R_{21} + R_{31} - R_{12} - R_{13} = 0$

Level 2: $R_{12} + R_{32} - R_{21} - R_{23} = 0$

Level 3: $R_{13} + R_{23} - R_{31} - R_{32} = 0$

where R_{ij} = rate of transitions from level i to level j

- Multiply each equation by level energy ε_1, ε_2, ε_3 and rearrange
  → obtain energy flow budget equations for each level's excitation pool

7.4.4 Energy Flow Rates and Macro Atom Equations

Translating statistical equilibrium into energy budgets for each level

Absorption Rates (radiation → excitation):

Energy flowing from radiation field into each excitation energy pool:

$$\dot{A}_{12} = \varepsilon_{12} R_{12}$$
$$\dot{A}_{13} = \varepsilon_{13} R_{13}$$
$$\dot{A}_{23} = \varepsilon_{23} R_{23}$$

($\varepsilon_{ij} = |\varepsilon_i - \varepsilon_j|$ = energy of the transition)

Emission Rates (excitation → radiation)

Energy flowing from each pool back to radiation:

$$\dot{E}_{21} = \varepsilon_{12} R_{21}$$
$$\dot{E}_{31} = \varepsilon_{13} R_{31}$$
$$\dot{E}_{32} = \varepsilon_{23} R_{32}$$

Energy Pool Balance Equations — [statistical eq. × level energies, rearranged]

Level 1: $\varepsilon_1 R_{21} + \varepsilon_1 R_{31} = \varepsilon_1 R_{12} + \varepsilon_1 R_{13}$ ($\varepsilon_1 = 0$ by convention, trivially satisfied)

Level 2: $\dot{A}_{12} + \varepsilon_1 R_{12} + \varepsilon_2 R_{32} = \dot{E}_{21} + \varepsilon_2 R_{23} + \varepsilon_1 R_{21}$

Level 3: $\dot{A}_{13} + \dot{A}_{23} + \varepsilon_1 R_{13} + \varepsilon_2 R_{23} = \dot{E}_{31} + \dot{E}_{32} + \varepsilon_2 R_{32} + \varepsilon_1 R_{31}$

source terms = sink terms for each level

$\dot{A}$ terms (LHS): radiation absorbed → realized as packet absorption events

$\dot{E}$ terms (RHS): radiation emitted → realized as packet emission events

$\varepsilon \cdot R$ terms: internal transitions — **each term appears twice: once in LHS of one equation, and once on RHS of another.**

Each term can be regarded as a source term for one level of the macro atom (appears together with absorption of radiation) and a sink term for another energy level.

Internal $\varepsilon \cdot R$ terms are viewed as internal (radiationless) transitions between levels of the excitation pools — the essence of the macro atom.

7.4.4 Macro Atom Algorithm

Traffic flow interpretation → Monte Carlo processing rules

(A) Activation - LHS

Whenever an active radiation packet is absorbed by any of the spectral lines,

→ interpret as realization of the corresponding $\dot{A}$ absorption term

→ The macro atom is said to be activated in the corresponding energy level

(B) Select Outcome - RHS

Inspect all sink terms on the RHS for the activated level; draw a random number ξ.

Select outcome with probability proportional to the energy flow rate.

Example (level 2): prob. $\dot{E}_{21}/D_2$ → emit in 2→1 transition (deactivation)

prob. $\varepsilon_2 R_{23}/D_2$ → internal transition 2→3 (stays active)

prob. $\varepsilon_1 R_{21}/D_2$ → internal transition 2→1 (stays active)

where $D_2 = \dot{E}_{21} + \varepsilon_2 R_{23} + \varepsilon_1 R_{21}$ (normalization factor)

(C-i) Deactivation

If an $\dot{E}$ (emission) term selected:

→ macro atom deactivates

→ packet returned to main MC simulation with new frequency and direction (sampled from the emission process)

→ packet energy ε conserved in the CMF (RE enforced)

(C-ii) Internal Transition

If an internal $\varepsilon \cdot R$ term selected:

→ macro atom remains active, switches state (e.g. selecting $\varepsilon_2 R_{23}/D_2$ results in "state 2→3")

→ return to step (B) and repeat

→ continue until a deactivation event (Ė term) is drawn

7.4.4 Key Properties of the Macro Atom Scheme

Important features, special cases, and computational considerations

Level Population Cancellation

All rates $R_{ij} \propto n_i$ (level population)

→ leading n_i dependence cancels in step (B) normalization

→ Macro atom transition probabilities can be computed without converged level populations!

Demonstrated for Fe II (Lucy 2002, Fig. 5)

Ground State Convention

$\varepsilon_1 = 0$ (standard zero of excitation energy)

→ No $\dot{A}$ or $\dot{E}$ terms for level 1

→ Internal $\varepsilon_1 \cdot R$ terms vanish

→ Simplifies algorithm: ground state excluded from explicit treatment

Special Cases — Both are limits of the full macro atom

- Effective resonance scattering: macro atom with only two levels, and $\varepsilon_1 = 0$
- Downbranching scheme (Lucy 1999b): macro atom with all internal $\varepsilon \cdot R$ transition terms suppressed (valid when downward rates dominate, and $\varepsilon_u \gg \varepsilon_l$)

Computational Efficiency

Repeated cycling (B)→(C-ii) can be costly for large atomic models.
Ergon et al. (2018): Markov-chain approach solves the macro atom without explicitly following internal state transitions → substantial reduction in computational cost.

- Note: Additional population dependence can re-enter via stimulated emission corrections and Sobolev escape probabilities (Sect. 8.2)

7.4.5 The Thermal Energy Pool (k-packets)

Extending the macro atom to include particle kinetic energy (Lucy 2002)

Generalize the macro atom to include the **thermal pool** of particle kinetic energies

Thermal Equilibrium (TE) Condition — Eq. (69):

$$H_{\mathrm{R}} + H_{\mathrm{C}} = C_{\mathrm{R}} + C_{\mathrm{C}}$$

H_{R} = radiative heating (e.g. free-free absorption) C_{R} = radiative cooling

H_{C} = collisional heating (de-excitation of atoms) C_{C} = collisional cooling (excitation)

k-packet Processing Algorithm

When a radiation packet is absorbed via a heating process (realizing H_{R} or H_{C}):

→ Energy flows into the thermal pool (a 'k-packet' event)

→ Sample all available cooling processes with probability proportional to their rates:

Prob. $C_{\mathrm{R}}/(C_{\mathrm{R}} + C_{\mathrm{C}})$: re-emit a radiation packet
(frequency and direction from cooling emissivity)

Prob. $C_{\mathrm{C}}/(C_{\mathrm{R}} + C_{\mathrm{C}})$: activate a macro atom at the collisionally excited level
(coupling thermal pool → excitation pool)

Cross-talk Between Pools

- Bound-free (photoionization/recombination) processes involve BOTH atomic and thermal pools simultaneously; handled by extending the traffic flow equations (Lucy 2003)
- Energy can cycle: radiation ↔ excitation pool ↔ thermal pool — all conserved exactly

7.5 Indivisible Energy Packets Beyond Radiative Equilibrium

Generalising to include external heating and non-equilibrium sinks

- When RE does not hold: add external source/sink terms to the energy balance equation

Generalised Energy Balance — [e.g. stellar outflow]:

$$H_{\mathrm{R}} + H_{\mathrm{C}} + H_{\mathrm{E}} = C_{\mathrm{R}} + C_{\mathrm{C}} + C_{\mathrm{E}}$$

H_{E} = external non-radiative heating (e.g. MHD heating) C_{E} = external cooling (adiabatic expansion)

Treating H_{E} (External Heating)

- H_{E} packets injected directly into the k-packet pool during the simulation
- Injection rate set by the external non-radiative process
- Energy initially enters as thermal kinetic energy
- Subsequently processed via the standard TE traffic flow rules (C_{R}, C_{C} channels)

Treating C_{E} (External Cooling / Sinks)

Option 1 — Packet Termination:
Prob. $C_{\mathrm{E}}/(C_{\mathrm{R}} + C_{\mathrm{C}} + C_{\mathrm{E}})$:
packet terminated (energy removed)

Option 2 — Energy Reduction:
Sample only C_{R}, C_{C} channels;
reduce packet energy by a factor accounting for expansion loss

Applications & Limiting Behaviour

- Adiabatic cooling implemented in: Long & Knigge 2002; Kasen et al. 2006; Kromer 2009; Vogl et al. 2019
- In the limit H_{E}, C_{E} dominant → reduces to the known-emissivity scheme of Sect. 7.1
- Extensions to non-statistical-equilibrium or non-TE terms not yet implemented (future work)

Summary: Chapter 7 — Emission Treatments in MCRT

Hierarchy from simple to general

7.1 Known Emissivity

- Emissivity given externally
- Direct sampling — no iteration
- Simple injection alongside other packets

7.2–7.3 RE by Iteration

- Iterative RT cycles
- Energy conservation only asymptotic
- Convergence issues at high τ

7.4 On-the-fly RE

- Indivisible energy packets
- Strict RE at every interaction
- Lucy 1999a, 2002, 2003

7.4.1–7.4.2

- Two-level: resonant scattering
- Redistribution parameter Λ
- Simple, fast; limited realism

7.4.3 Downbranching

- q_{u→l} ∝ energy flow rates
- Multi-level downward only
- Excellent for SN Ia spectra

7.4.3–7.4.4 Macro Atom

- All transitions (up + down)
- Level pops cancel from rates
- Most complete treatment

7.4.5 k-packets

- Thermal energy pool added
- $H_{\mathrm{R}} + H_{\mathrm{C}} = C_{\mathrm{R}} + C_{\mathrm{C}}$ (TE)
- Couples to macro atom

7.5 Beyond RE

- External H_{E}, C_{E} terms
- Packet termination / reduction
- Adiabatic cooling in SNe codes

Key Achievement

- Level pops cancel → no need for converged populations
- Macro atom = general framework

Monte Carlo Radiative Transfer Algorithm in a Uniform-Density Sphere

Outline

Goal

- Emit N_{ph} photon packets inside a uniform-density sphere of optical radius R.
- Each packet propagates until it
  - escapes through the outer boundary, or
  - is absorbed inside the medium.
- Along the way it may undergo scattering events.

Escape fraction

$$f_{\mathrm{esc}} = \frac{N_{\mathrm{esc}}}{N_{\mathrm{ph}}}$$

Optical-depth units

All distances are measured in optical-depth units.

$$\chi = \rho\,\kappa_{\mathrm{ext}}, \qquad R \equiv \tau_R = \chi\,R_{\mathrm{phys}}.$$

Hence R, the position $\boldsymbol{r}$, the flight distance ℓ, and the sampled interaction optical depth τ are all dimensionless.

In physical coordinates, the distance to the next interaction is

$$s = \frac{-\ln\xi}{\chi},$$

and the sphere radius is R_{phys}.

Notation and parameters

Symbol	Meaning
N_{ph}	Number of photon packets
R	Optical radius of the sphere
a	Single-scattering albedo
ξ	Independent uniform random number on $[0,1]$
$\boldsymbol{r}$	Current photon-packet position
$\hat{\boldsymbol{k}}$	Current propagation direction
N_{esc}	Number of escaped packets
N_{abs}	Number of absorbed packets

$$a = \frac{\chi_{\mathrm{sca}}}{\chi_{\mathrm{abs}} + \chi_{\mathrm{sca}}}.$$

- At an interaction: scatter with prob. a, absorb with prob. $1-a$.
- $a = 1$: pure scattering — every packet eventually escapes.

Sampling the initial position

Volume element $\mathrm{d}V = r^2 \sin\theta \, \mathrm{d}r \, \mathrm{d}\theta \, \mathrm{d}\phi$ gives

$$P(< r) = \frac{r^3}{R^3} \quad \Longrightarrow \quad r = R\xi_1^{1/3}.$$

Angular variables (uniform on the sphere):

$$\mu = \cos\theta = 2\xi_2 - 1, \qquad \phi = 2\pi\xi_3.$$

$$\boldsymbol{r}_0 = \left(r\sqrt{1-\mu^2}\cos\phi,\ r\sqrt{1-\mu^2}\sin\phi,\ r\mu\right).$$

Key point

Sample $\mu = \cos\theta$ uniformly — not θ itself.

Sampling the initial direction (isotropic)

Same recipe as a random direction on the unit sphere:

$$\mu_k = 2\xi_4 - 1, \qquad \phi_k = 2\pi\xi_5.$$

$$\hat{\boldsymbol{k}} = \left(\sqrt{1-\mu_k^2}\cos\phi_k,\ \sqrt{1-\mu_k^2}\sin\phi_k,\ \mu_k\right).$$

Initial position and initial direction are assumed independent. For a central source, an external incident beam, or a beamed source, only this initialisation step changes.

Optical depth to the next interaction

In a uniform medium, the optical depth to the next extinction event is exponentially distributed:

$$\tau_{\text{int}} = -\ln \xi \,.$$

Compare with ℓ_{esc}, the optical distance to the boundary along $\hat{\boldsymbol{k}}$:

- $\tau_{\text{int}} \geq \ell_{\text{esc}} \implies$ packet reaches the boundary first *(escape)*.
- $\tau_{\text{int}} < \ell_{\text{esc}} \implies$ packet interacts inside the sphere.

Distance to the sphere boundary

Boundary: $|\boldsymbol{r}|^2 = R^2$. After a step ℓ along $\hat{\boldsymbol{k}}$,

$$|\boldsymbol{r} + \ell\hat{\boldsymbol{k}}|^2 = R^2 \quad \Longrightarrow \quad \ell^2 + 2(\boldsymbol{r}\cdot\hat{\boldsymbol{k}})\,\ell + (|\boldsymbol{r}|^2 - R^2) = 0.$$

Positive root for a packet inside the sphere:

$$\boxed{\ell_{\mathrm{esc}} \;=\; -\boldsymbol{r}\cdot\hat{\boldsymbol{k}} + \sqrt{(\boldsymbol{r}\cdot\hat{\boldsymbol{k}})^2 + R^2 - |\boldsymbol{r}|^2}\,.}$$

Escape point on the boundary:

$$\boldsymbol{r}_{\mathrm{esc}} \;=\; \boldsymbol{r} + \ell_{\mathrm{esc}}\,\hat{\boldsymbol{k}}.$$

Interaction handling

If $\tau_{\text{int}} < \ell_{\text{esc}}$, update the position:

$$\boldsymbol{r} \leftarrow \boldsymbol{r} + \tau_{\text{int}} \hat{\boldsymbol{k}}.$$

Then draw a fresh ξ:

$$\xi \le a \implies \text{scattering}, \qquad \xi > a \implies \text{absorption}.$$

- **Absorption**: terminate the packet, increment N_{abs}.
- **Scattering**: sample a new propagation direction and continue tracking.

Scattering: sample the angles in the local frame

Phase function $p(\cos\theta_s)$ gives the density of the scattering angle between the incoming $\hat{\boldsymbol{k}}$ and outgoing $\hat{\boldsymbol{k}}'$. Sample

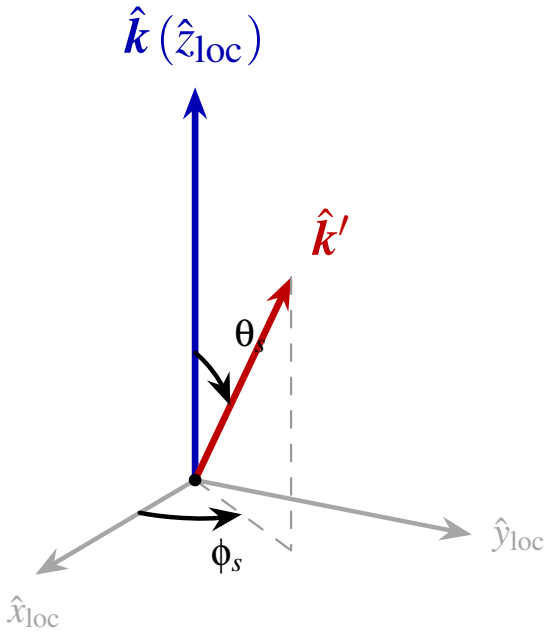
$$\mu_s = \cos\theta_s \sim p(\mu_s), \qquad \phi_s = 2\pi\xi\,.$$

- **Isotropic:** $p(\mu_s) = \frac{1}{2}$, so $\mu_s = 2\xi - 1$.
- **Henyey–Greenstein** $(g \in (-1,1))$:

$$p_{\mathrm{HG}}(\mu_s) = \frac{1-g^2}{2(1+g^2-2g\mu_s)^{3/2}},$$

$$\mu_s = \frac{1}{2g}\left[1+g^2-\left(\frac{1-g^2}{1-g+2g\xi}\right)^2\right] \quad (g \neq 0).$$

Scattering geometry in the local frame



Local frame: $\hat{z}_{\mathrm{loc}} = \hat{\boldsymbol{k}}$. Sample (θ_s, ϕ_s) about $\hat{\boldsymbol{k}}$.

$$\hat{\boldsymbol{k}}'_{\mathrm{local}} = \begin{pmatrix} \sin\theta_s \cos\phi_s \\ \sin\theta_s \sin\phi_s \\ \cos\theta_s \end{pmatrix}.$$

To get the global-frame direction, apply the rotation that maps the local $\hat{z}$ onto $\hat{\boldsymbol{k}}$ (next slide).

Scattering: rotation to the global frame

Apply $R = R_z(\Phi)\,R_y(\Theta)$ with $\cos\Theta = k_z$, $S \equiv \sin\Theta = \sqrt{1-k_z^2}$, $\cos\Phi = k_x/S$, $\sin\Phi = k_y/S$.

General case $(S > \varepsilon)$:

$$k_x' = \frac{\sin\theta_s\,(k_x k_z \cos\phi_s - k_y \sin\phi_s)}{S} + k_x\cos\theta_s,$$

$$k_y' = \frac{\sin\theta_s\,(k_y k_z \cos\phi_s + k_x \sin\phi_s)}{S} + k_y\cos\theta_s,$$

$$k_z' = -S\sin\theta_s\cos\phi_s + k_z\cos\theta_s.$$

Degenerate case ($\hat{\boldsymbol{k}} \approx \pm\hat{z}$, choose $\Phi = 0$):

$$k_x' = \sin\theta_s\cos\phi_s, \quad k_y' = \sin\theta_s\sin\phi_s, \quad k_z' = \mathrm{sgn}(k_z)\cos\theta_s.$$

Update $\hat{\boldsymbol{k}} \leftarrow \hat{\boldsymbol{k}}'/|\hat{\boldsymbol{k}}'|$.

Isotropic scattering as a special case

For $p(\mu_s) = \frac{1}{2}$, the rotated direction $\hat{\boldsymbol{k}}'$ is uniform over the full sphere regardless of $\hat{\boldsymbol{k}}$.

Shortcut

Skip the rotation and sample $\hat{\boldsymbol{k}}'$ directly in the global frame:

$$\mu' = 2\xi_1 - 1, \quad \phi' = 2\pi\xi_2,$$

$$\hat{\boldsymbol{k}}' = \left(\sqrt{1-(\mu')^2}\cos\phi',\ \sqrt{1-(\mu')^2}\sin\phi',\ \mu'\right).$$

For any anisotropic phase function the rotation is required.

Complete algorithm (1/2): scatter direction

```
Input:  N_ph, R, a
Output: f_esc and its Monte Carlo uncertainty

N_esc = 0; N_abs = 0

# Rotate a locally-sampled scattered direction (mu_s, phi_s)
# from the local frame about k into the global frame.
function scatter_direction(k, mu_s, phi_s):
    sin_ts = sqrt(1 - mu_s^2)
    S = sqrt(k[0]^2 + k[1]^2)            # = sqrt(1 - k[2]^2)
    if S > eps:
        kp[0] = sin_ts*(k[0]*k[2]*cos(phi_s) - k[1]*sin(phi_s))/S
                                                    + k[0]*mu_s
        kp[1] = sin_ts*(k[1]*k[2]*cos(phi_s) + k[0]*sin(phi_s))/S
                                                    + k[1]*mu_s
        kp[2] = -S*sin_ts*cos(phi_s) + k[2]*mu_s
    else:                                # k nearly along +/-z axis
        kp[0] = sin_ts*cos(phi_s)
        kp[1] = sin_ts*sin(phi_s)
        kp[2] = sign(k[2])*mu_s
    return normalize(kp)
```

Complete algorithm (2/2): main loop

```
for n = 1, ..., N_ph:
    r = sample_uniform_position_in_sphere(R)
    k = sample_isotropic_direction()
    while photon is alive:
        tau_int = -log(U())
        b       = dot(r, k)
        ell_esc = -b + sqrt(b*b + R*R - dot(r, r))
        if tau_int >= ell_esc:                      # escape
            r_escape = r + ell_esc*k
            N_esc += 1
            terminate this photon
        else:                                       # interaction
            r = r + tau_int*k
            if U() <= a:                            # scattering
                mu_s  = sample_phase_function()     # 2*U()-1 if iso
                phi_s = 2*pi*U()
                k = scatter_direction(k, mu_s, phi_s)
                continue
            else:                                   # absorption
                N_abs += 1
                terminate this photon

f_esc   = N_esc / N_ph
sigma_f = sqrt(f_esc*(1 - f_esc)/N_ph)
```

Estimating the escape fraction

Indicator variable:

$$X_i = \begin{cases} 1, & \text{packet } i \text{ escapes} \\ 0, & \text{absorbed} \end{cases}$$

Estimator:

$$\widehat{f}_{\mathrm{esc}} = \frac{1}{N_{\mathrm{ph}}} \sum_{i=1}^{N_{\mathrm{ph}}} X_i = \frac{N_{\mathrm{esc}}}{N_{\mathrm{ph}}}, \qquad \widehat{f}_{\mathrm{abs}} = 1 - \widehat{f}_{\mathrm{esc}}.$$

Binomial standard error (independent packets):

$$\sigma\left(\widehat{f}_{\mathrm{esc}}\right) = \sqrt{\frac{\widehat{f}_{\mathrm{esc}}\left(1 - \widehat{f}_{\mathrm{esc}}\right)}{N_{\mathrm{ph}}}}.$$

- Report $f_{\mathrm{esc}} = \widehat{f}_{\mathrm{esc}} \pm \sigma\left(\widehat{f}_{\mathrm{esc}}\right)$.
- Near 0 or 1: use a Wilson interval or Bayesian beta interval.

Escape fraction vs. optical depth

Repeat for a sequence $R_1, R_2, \ldots, R_m$ and obtain

$$\left\{R_j, \widehat{f}_{\mathrm{esc}}(R_j, a),\ \sigma_j\right\}_{j=1}^{m}.$$

- Smaller R: packets escape easily.
- Larger R: more interactions $\Rightarrow$ more absorption (if $a < 1$) $\Rightarrow f_{\mathrm{esc}}$ decreases.
- $a = 1$: $f_{\mathrm{esc}} = 1$ for any finite R, but the number of scatterings can be very large.

Implementation notes

- **Pure-scattering check** ($a = 1$): expect $N_{\text{esc}} = N_{\text{ph}}$ for sufficient iteration limit.
- **Pure-absorption check** ($a = 0$): per initial condition,

$$P_{\text{esc}}(\boldsymbol{r}, \hat{\boldsymbol{k}}) = e^{-\ell_{\text{esc}}}.$$

  Monte Carlo result should converge to its average over initial conditions.
- **Independent random numbers**: never reuse a single draw across position, direction, distance, and event-type sampling.
- **Angular sampling**: sample $\mu = \cos\theta$ uniformly, not θ.
- **Roundoff**: occasionally renormalise $\hat{\boldsymbol{k}}$; use a small tolerance near $|\boldsymbol{r}|^2 = R^2$.
- **Iteration cap**: photons that hit a maximum-scattering limit should be recorded *separately*, not counted as absorbed.

Summary

- Monte Carlo recipe for the escape fraction $f_{\mathrm{esc}}(R, a)$ of a uniform sphere.
- Per-photon loop: sample distance $\tau_{\mathrm{int}} = -\ln \xi$, test against ℓ_{esc}, then scatter or absorb.
- Direction update: sample (θ_s, ϕ_s) in the local frame along $\hat{\boldsymbol{k}}$, then rotate to the global frame.
- Report

$$f_{\mathrm{esc}} = \widehat{f}_{\mathrm{esc}} \pm \sigma(\widehat{f}_{\mathrm{esc}}), \qquad \sigma = \sqrt{\widehat{f}_{\mathrm{esc}}(1 - \widehat{f}_{\mathrm{esc}})/N_{\mathrm{ph}}}.$$

Monte Carlo Radiative Transfer: Thomson Scattering Spectrum in a Uniform-Density Sphere

Outline

Goal

- N_{ph} photon packets emitted at frequency ν_0 from the *centre* of a uniform sphere of optical radius R.
- Pure-scattering medium: free electrons with Maxwell–Boltzmann velocities at temperature T.
- Each scattering shifts the frequency via the thermal Doppler effect.
- Track the normalized frequency $q \equiv \nu/\nu_0$ until each packet escapes; estimate the spectrum $S(q)$.

$$R \equiv n_e\, \sigma_T\, R_{\mathrm{phys}}, \qquad q\big|_{\mathrm{initial}} = 1.$$

Notation and parameters

Symbol	Meaning
N_{ph}	Number of photon packets
R	Optical radius of the sphere
T	Electron temperature
σ_v	1D thermal speed, $\sigma_v = \sqrt{k_B T / m_e}$
q	Normalized frequency, $q = \nu / \nu_0$
ξ	Independent uniform random number on $[0, 1]$
$\boldsymbol{r}$	Photon-packet position
$\hat{\boldsymbol{k}}$	Propagation direction
N_{esc}	Number of escaped photon packets

Non-relativistic gas: keep first-order v/c; higher-order corrections and photon recoil are neglected.

Initial position, direction, and frequency

Position: all packets emitted from the centre,

$$\boldsymbol{r}_0 = 0.$$

Direction: isotropic,

$$\mu_k = 2\xi_1 - 1, \qquad \phi_k = 2\pi\xi_2,$$

$$\hat{\boldsymbol{k}} = \left(\sqrt{1-\mu_k^2}\cos\phi_k,\ \sqrt{1-\mu_k^2}\sin\phi_k,\ \mu_k\right).$$

Frequency: $q = 1$.

Distance to next scattering and to the boundary

Optical depth to next scattering (uniform medium):

$$\tau_{\rm int} = -\ln \xi \,.$$

Distance to boundary along $\hat{\boldsymbol{k}}$ (positive root of $|\boldsymbol{r} + \ell\hat{\boldsymbol{k}}|^2 = R^2$):

$$\ell_{\rm esc} = -\boldsymbol{r}\cdot\hat{\boldsymbol{k}} + \sqrt{(\boldsymbol{r}\cdot\hat{\boldsymbol{k}})^2 + R^2 - |\boldsymbol{r}|^2}\,.$$

- $\tau_{\rm int} \geq \ell_{\rm esc} \implies$ photon escapes (record q).
- $\tau_{\rm int} < \ell_{\rm esc} \implies$ move to interaction site, scatter.

Thomson phase function

Unpolarised Thomson scattering: $\propto 1+\cos^2\theta_s$. Normalised:

$$p(\mu_s) = \frac{3}{8}\left(1+\mu_s^2\right), \qquad \mu_s \equiv \cos\theta_s \in [-1,1].$$

$$\int_{-1}^{1} \frac{3}{8}(1+\mu_s^2)\,\mathrm{d}\mu_s = 1.$$

- Symmetric about $\mu_s = 0$: equal forward / backward weight.
- Suppressed at $\mu_s = 0$ (right-angle scattering minimum).

Sampling μ_s by superposition

Decompose

$$p(\mu_s) = w_1\, p_1(\mu_s) + w_2\, p_2(\mu_s),$$

with

$$w_1 = \tfrac{3}{4},\ \ p_1(\mu_s) = \tfrac{1}{2}\ \text{(isotropic)}, \qquad w_2 = \tfrac{1}{4},\ \ p_2(\mu_s) = \tfrac{3}{2}\mu_s^2.$$

Inversions:

$$p_1\colon\ \ \mu_s = 2\xi - 1, \qquad p_2\colon\ \ \mu_s = (2\xi-1)^{1/3}\ \text{(signed cube root)}.$$

Procedure

- If $\xi_1 < 3/4$: $\mu_s = 2\xi_2 - 1$.
- Else: $\mu_s = \operatorname{sgn}(2\xi_2 - 1)\,|2\xi_2 - 1|^{1/3}$.

Then $\sin\theta_s = \sqrt{1-\mu_s^2}$, $\phi_s = 2\pi\xi_3$.

Scattering rate in the electron rest frame

Decompose electron velocity in $\{\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_2, \hat{\boldsymbol{k}}\}$:

$$\vec{v} = v_{\parallel}\hat{\boldsymbol{k}} + v_{\perp,1}\hat{\boldsymbol{e}}_1 + v_{\perp,2}\hat{\boldsymbol{e}}_2.$$

Each component is $\mathcal{N}(0, \sigma_v^2)$.

Differential rate (rest-frame view):

$$\mathrm{d}\Gamma \propto \underbrace{c}_{\text{photon flux}} \times \underbrace{\sigma(\nu_e)}_{\text{cross section}} \times \underbrace{f_1(v_{\parallel}) f_1(v_{\perp,1}) f_1(v_{\perp,2})\, \mathrm{d}^3 v}_{\text{electron number density}}.$$

To first order,

$$\nu_e = \nu\left(1 - \frac{v_{\parallel}}{c}\right),$$

so only $v_{\parallel}$ enters the cross-section.

Sampling the velocity components

Transverse $v_{\perp,1}, v_{\perp,2}$: always unweighted Maxwell,

$$v_{\perp,1},\ v_{\perp,2} \sim \mathcal{N}(0, \sigma_v^2).$$

Parallel $v_{\parallel}$: cross-section-weighted Maxwell,

$$P(v_{\parallel}) \propto \sigma\big(\nu(1 - v_{\parallel}/c)\big) f_1(v_{\parallel}).$$

Thomson special case

$\sigma(\nu_e) = \sigma_T = \text{const}$ so the cross-section factor drops out, and $v_{\parallel} \sim \mathcal{N}(0, \sigma_v^2)$ as well — all three components Gaussian.

Frequency shift after a scattering

With the outgoing direction

$$\hat{\boldsymbol{k}}' = \sin\theta_s \cos\phi_s \, \hat{\boldsymbol{e}}_1 + \sin\theta_s \sin\phi_s \, \hat{\boldsymbol{e}}_2 + \mu_s \hat{\boldsymbol{k}},$$

the first-order Doppler shift is

$$\Delta \equiv \frac{\nu' - \nu}{\nu} = \frac{(\hat{\boldsymbol{k}}' - \hat{\boldsymbol{k}}) \cdot \vec{v}}{c}.$$

$$\Delta = \frac{v_{\parallel}(\mu_s - 1) + \sin\theta_s \left(v_{\perp,1} \cos\phi_s + v_{\perp,2} \sin\phi_s \right)}{c}.$$

Forward scattering ($\mu_s = 1$): $\Delta = 0$.

Thomson: Gaussian sampling of Δ

All three velocity components Gaussian $\Rightarrow$ Δ is zero-mean Gaussian:

$$\mathrm{Var}(\Delta) = \frac{\sigma_v^2}{c^2}\left[(\mu_s - 1)^2 + \sin^2\theta_s\right] = \frac{2\sigma_v^2(1-\mu_s)}{c^2}.$$

Sample

$$\Delta = \frac{\sigma_v}{c}\sqrt{2(1-\mu_s)}\,Z, \qquad Z \sim \mathcal{N}(0,1).$$

Box–Muller:

$$Z = \sqrt{-2\ln\xi_4}\,\cos(2\pi\xi_5).$$

Update:

$$q \leftarrow q(1+\Delta), \qquad q_n = \prod_{i=1}^{n}(1+\Delta_i).$$

Rotation to the global frame

Apply the rotation that maps the local $\hat{z}$ to $\hat{\boldsymbol{k}}$. Let $S = \sqrt{1 - k_z^2}$.

General case ($S > \varepsilon$):

$$k'_x = \frac{\sin\theta_s \left(k_x k_z \cos\phi_s - k_y \sin\phi_s\right)}{S} + k_x \mu_s,$$

$$k'_y = \frac{\sin\theta_s \left(k_y k_z \cos\phi_s + k_x \sin\phi_s\right)}{S} + k_y \mu_s,$$

$$k'_z = -S \sin\theta_s \cos\phi_s + k_z \mu_s.$$

Degenerate ($\hat{\boldsymbol{k}} \approx \pm\hat{z}$):

$$k'_x = \sin\theta_s \cos\phi_s, \quad k'_y = \sin\theta_s \sin\phi_s, \quad k'_z = \mathrm{sgn}(k_z)\, \mu_s.$$

Renormalise: $\hat{\boldsymbol{k}} \leftarrow \hat{\boldsymbol{k}}' / |\hat{\boldsymbol{k}}'|$.

Spectral estimation

N_{bin} uniform bins on $[q_{\min}, q_{\max}]$, width $\Delta q = (q_{\max} - q_{\min})/N_{\mathrm{bin}}$.
At each escape, increment

$$H[j], \qquad j = \left\lfloor \frac{q - q_{\min}}{\Delta q} \right\rfloor .$$

Spectrum estimator:

$$\widehat{S}(q_j) = \frac{H[j]}{N_{\mathrm{ph}}\,\Delta q}, \qquad q_j = q_{\min} + \left(j + \tfrac{1}{2}\right)\Delta q.$$

Per-bin Monte Carlo error:

$$\sigma_j = \frac{\sqrt{H[j]}}{N_{\mathrm{ph}}\,\Delta q}.$$

Normalisation (no absorption): $\sum_j \widehat{S}(q_j)\Delta q \xrightarrow{N_{\mathrm{ph}}\to\infty} 1$.

Complete algorithm (1/2): helper functions

```
Input:  N_ph, R, sigma_v, c, q_min, q_max, N_bin
Output: spectrum S[0..N_bin-1] and uncertainty sigma[0..N_bin-1]

dq = (q_max - q_min) / N_bin
H[0..N_bin-1] = 0;  N_esc = 0

function sample_thomson_angle():
    if U() < 0.75:
        mu_s = 2*U() - 1                # isotropic: p1
    else:
        mu_s = cbrt(2*U() - 1)          # cosine-squared: p2
    return mu_s

function scatter_direction(k, mu_s, phi_s):
    sin_ts = sqrt(1 - mu_s^2)
    S = sqrt(k[0]^2 + k[1]^2)
    if S > eps:
        kp[0] = sin_ts*(k[0]*k[2]*cos(phi_s) - k[1]*sin(phi_s))/S + k[0]*mu_s
        kp[1] = sin_ts*(k[1]*k[2]*cos(phi_s) + k[0]*sin(phi_s))/S + k[1]*mu_s
        kp[2] = -S*sin_ts*cos(phi_s) + k[2]*mu_s
    else:
        kp[0] = sin_ts*cos(phi_s)
        kp[1] = sin_ts*sin(phi_s)
        kp[2] = sign(k[2])*mu_s
    return normalize(kp)

function box_muller():                  # returns Z ~ N(0,1)
    return sqrt(-2*log(U())) * cos(2*pi*U())
```

Complete algorithm (2/2): main loop

```
for n = 1, ..., N_ph:
    r = (0, 0, 0)
    k = sample_isotropic_direction()    # mu_k = 2*U()-1, phi_k = 2*pi*U()
    q = 1.0
    while photon has not escaped:
        tau_int = -log(U())
        b       = dot(r, k)
        l_esc   = -b + sqrt(b*b + R*R - dot(r,r))
        if tau_int >= l_esc:            # photon escapes
            N_esc += 1
            j = floor((q - q_min) / dq)
            if 0 <= j < N_bin:
                H[j] += 1
            break
        else:                           # scattering inside sphere
            r     = r + tau_int * k
            mu_s  = sample_thomson_angle()
            phi_s = 2*pi*U()
            Z     = box_muller()
            delta = (sigma_v/c) * sqrt(2*(1 - mu_s)) * Z
            q     = q * (1 + delta)
            k     = scatter_direction(k, mu_s, phi_s)

for j = 0, ..., N_bin-1:
    S[j]     = H[j] / (N_ph * dq)
    sigma[j] = sqrt(H[j]) / (N_ph * dq)
```

Single-scattering width and other checks

- **Phase-function check**: histogram μ_s and recover $p(\mu_s) = \frac{3}{8}(1+\mu_s^2)$: a flat background plus a μ_s^2 peak at ± 1.
- **Single-scattering width** (optically thin, $R \ll 1$):

$$\langle 1-\mu_s \rangle_{\mathrm{Th}} = \int_{-1}^{1} (1-\mu_s)\frac{3}{8}(1+\mu_s^2)\,\mathrm{d}\mu_s = \frac{13}{16},$$

$$\mathrm{Var}(\Delta) = \frac{2\sigma_v^2}{c^2}\langle 1-\mu_s \rangle_{\mathrm{Th}}, \quad \sigma_q \approx \sqrt{13/8}\,\frac{\sigma_v}{c} \approx 1.27\,\frac{\sigma_v}{c}.$$

- **Zero-shift symmetry**: Maxwell–Boltzmann symmetric in $\vec{v} \Rightarrow \langle \Delta \rangle = 0$ per scattering. A net shift requires $\mathscr{O}(v^2/c^2)$.
- **Cold-electron limit** ($\sigma_v \to 0$): $S(q) \to \delta(q-1)$ (single bin).
- **Cube root**: in Fortran use $\mathrm{sgn}(u)\,|u|^{1/3}$; $u^{1/3}$ for $u<0$ is undefined.
- **Box–Muller guard**: avoid $\xi = 0$ (positive floor or zero-excluding generator).
- **Iteration cap**: record capped photons *separately*, do not discard.

Summary

- Monte Carlo recipe for the Thomson scattering spectrum from a uniform sphere of optical radius R at electron temperature T.
- Phase function $\propto 1+\mu_s^2$, sampled by superposition of an isotropic (p_1) and a cosine-squared (p_2) component.
- Per scattering: sample three Gaussian velocity components and apply

$$\Delta = \frac{\sigma_v}{c}\sqrt{2(1-\mu_s)}\,Z, \qquad q \leftarrow q\,(1+\Delta).$$

- Spectrum from histogrammed escape q:

$$\widehat{S}(q_j) = \frac{H[j]}{N_{\mathrm{ph}}\,\Delta q}, \qquad \sigma_q^{1\,\mathrm{scat}} \approx 1.27\,\frac{\sigma_v}{c}.$$