복사전달 특강

Special Topics in Radiative Transfer

Lecture 11 & 12

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Based on: Chapter 9 of Noebauer & Sim (Living Reviews in Computational Astrophysics)

선광일 (Kwangil Seon)

KASI / UST

Chapter 9: Extracting Information from MCRT Simulations

MC noise, direct counting, volume-based estimators, and biasing

Individual packet trajectories are not of primary interest — we need **ensemble averages**

Extracting accurate physical quantities requires dealing with the inherent **MC noise**

- In some cases, only radiation escaping from the simulation box is of interest to construct synthetic spectra, light curves or images.
- For other applications, it is required to characterize the radiation field internal to the system.
- Three main strategies presented in this chapter:

9.1 MC Noise

- Fundamental stochastic property
- $\sigma \propto N^{-1/2}$ (central limit theorem)
- Motivates all extraction techniques

9.2–9.3 Estimators

- Direct counting: simple but noisy
- Volume-based estimators (Lucy 1999a): use full trajectory history
- Much less noise for same N

9.4 Biasing

- Importance sampling: invest effort where it matters
- Biased emission, forced scattering, peel-off
- Russian Roulette + composite biasing

9.1 Monte Carlo Noise

The fundamental stochastic fluctuation inherent to all MC calculations

MCRT simulations are **probabilistic**: any quantity extracted will carry stochastic fluctuations

This is called **MC noise** — it is unavoidable but can be reduced by increasing N or using smarter estimators

- The **law of large numbers** guarantees convergence; the central limit theorem quantifies the noise

MC Estimator (Eq. 90): $G_N = \frac{1}{N}\sum_{i=1}^{N} X_i$ → converges to $E[X]$ as $N \to \infty$

Standard error (Eq. 91): $\sigma_G = \sigma_X/\sqrt{N}$

→ To halve the noise, one must use FOUR TIMES as many packets!

Implications for MCRT Design

- Simple estimates require enormous N for high accuracy
- Noise reduction is a primary driver of algorithm development
- Techniques should maximize the number of useful contributions — ***These methods are often referred to as acceleration techniques since they achieve a certain S/N level with fewer quanta.***
- A 'useful contribution' is one that informs the quantity of interest

Example: Escape Probability from a Sphere

- Experiment: packet escapes (X=1) or not (X=0)
- G_N → escape probability with N packets
- $\sigma_G = \sigma_X/\sqrt{N}$ (Fig. 11 demonstrates this)
- High-accuracy result needs $N \sim 10^5 - 10^6$

9.1 MC Noise Scaling: σ ∝ N^{−1/2}

Fig. 11 — Standard error vs number of MC packets

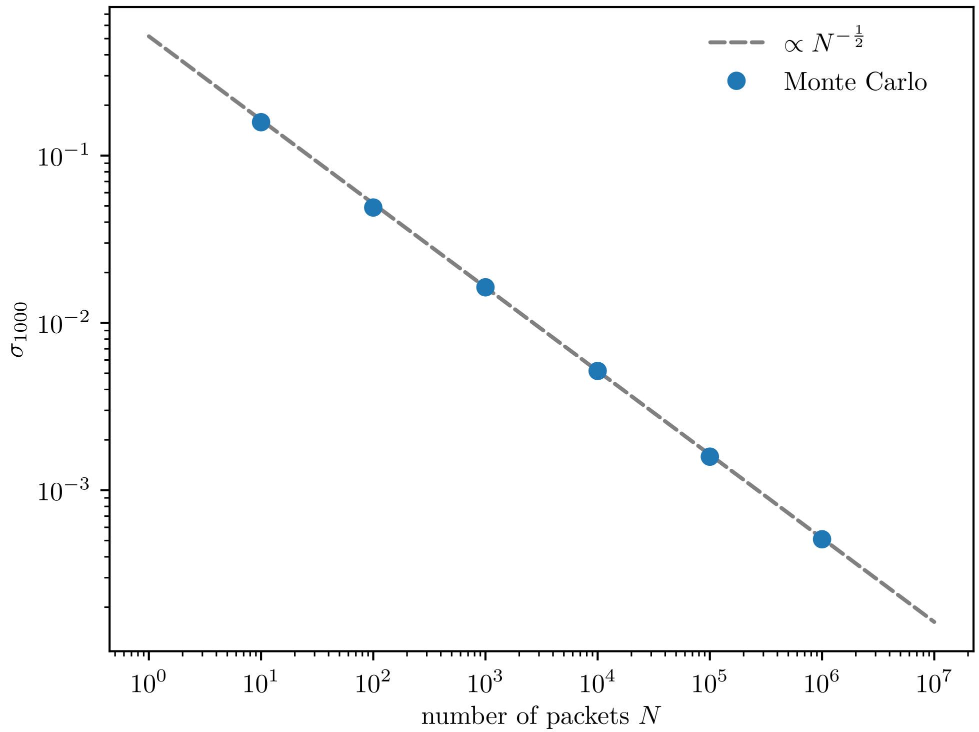

Fig. 11: Standard error σ_{1000} (estimated from 1000 repeated experiments) for the escape probability from a homogeneous sphere (τ_{sp} = 1) as a function of the number of packets N. The result follows $\sigma \propto N^{-1/2}$ (dashed line) almost perfectly, confirming the central limit theorem behavior.

Key takeaway: accuracy improves slowly with N ($\sigma \propto N^{-1/2}$).
Volume-based estimators and biasing achieve much better accuracy for the same cost.

9.2 Direct Counting of Packets

The simplest — and noisiest — reconstruction approach

Direct counting:

- From the ensemble of packet trajectories, simply count the relevant packet properties or packet interaction events.
- Most natural approach: simple to implement, intuitive, and sometimes sufficient
- Limitation: relies on packets being at the right place at the right time

Synthetic Image

$$L(\Delta S_i, \Delta\Omega_j) = \frac{1}{\Delta t} \sum_k \varepsilon_k$$

- Sum over packets escaping through surface element ΔS_i into solid angle element $\Delta\Omega_j$ during a time interval Δt
- Natural for synthetic spectra and images

Internal Energy Density

$$E_i = \frac{1}{\Delta V_i} \sum_j \varepsilon_j$$

- Sum over all packets (j) inside grid cell i at time $t = t^n$
- Radiation-matter interaction: The amount of absorbed radiant energy can be determined by counting all absorptions packets perform during a certain time interval.
- Requires many packets in each cell → can be very noisy

- In general, a large number of packets will be needed to achieve acceptable results since the approach requires that a sufficient number of packets propagate into the desired direction, are at a certain location or have performed a particular interaction.
- Still useful as a **reference/validation** for more sophisticated estimators
- The quality of direct counting estimates can be vastly improved when combined with biasing techniques.

9.3 Volume-Based Estimators (VBEs)— Concept

Lucy (1999a): use trajectory information instead of instantaneous snapshots

Key idea: instead of snapshots, use the **full trajectory** of each packet through each cell

- A packet that traverses a cell contributes information to ALL cells along its path — not just one
- This dramatically increases the number of contributions per cell → much lower noise

In direct counting approach, a momentary snapshot of the packet distribution is used.

Volume-Based Estimator principle (Lucy 1999a):

Each trajectory segment j of length l_j (in cell ΔV_j) contributes to the estimator weighted by $l_j / c\Delta t$.

→ Both forward-scattered AND backscattered contributions are included!

Advantages Over Direct Counting

- A single packet contributes to multiple cells
- Backscattered packets also contribute (can re-enter a cell)
- Non-zero result as long as ANY packet passed through the cell
- Especially powerful in optically thin regions

Physical Basis

- The specific intensity is an integral over angle
- Packet trajectory elements statistically represent the radiation field
- Time-averaged properties are more stable than snapshots
- Applicable to both time-dependent and steady-state RT

9.3.1 Example: Energy Density Estimator

Deriving the volume-based estimator for the radiation energy density

- Consider a packet with energy ε propagating in cell ΔV_i during simulation time step Δt
- The packet spends time δt_j on segment j. Each packet trajectory segment contributes to the total energy content with its packet energy, weighted by the relative time spent on that trajectory: $\Delta E = (\delta t_j / \Delta t) \cdot \varepsilon_j$.
- Thus, the total energy density for a grid cell i of volume ΔV_i may be constructed from an estimator obtained by summing over all trajectory elements of all packets that were active in the cell:

Time-based estimator: $E_i = \frac{1}{\Delta V_i} \sum_{j \in \Delta V_i} \frac{\delta t_j}{\Delta t} \varepsilon_j$ (The summation includes the trajectory segments j of all packets that lie within the cell i.)

Since packets travel at speed c, the estimator can be expressed in terms of trajectory segment length $l = c\delta t$.

→ Length-based estimator: $E_i = \frac{1}{\Delta t c \Delta V_i} \sum_{j \in \Delta V_i} l_j \varepsilon_j \quad \Leftarrow \quad \text{Normalization}: \quad L = \frac{1}{\Delta t} \sum_{k=1}^{N_{\text{ph}}} \varepsilon_k$

Key Properties

- Sum includes ALL trajectory segments in cell ΔV_i (physical scatterings AND numerical events like cell crossings)
- The ratio $\varepsilon_i / \Delta t$ is independent of the absolute time interval
  → Applicable to time-independent steady-state problems!

Practical Implementation

- During propagation loop: at each segment, add $l_j \varepsilon_j$ to cell estimator
- After simulation: divide by $\Delta t \cdot c \cdot \Delta V_i$
- For time-independent: Δt cancels out (only ratios matter)
- Easily extended to other radiation field quantities

9.3.2 Constructing VBEs: Radiation Field Quantities

Estimators for mean intensity J, flux H (or F), and second moment K

Using $E = (4\pi/c)J$ and the volume-based estimator for E:

Mean Intensity J_i

$$J_i = \frac{1}{4\pi \Delta V_i \Delta t} \sum_{j \in \Delta V_i} l_j \varepsilon_j$$

- Restrict sum to segments in direction $\Delta\Omega_k$ → specific intensity $I_j(\Omega_k)$
- Further restrict by frequency interval → monochromatic $I_j(\Omega_k, \nu_p)$

Radiation Flux F_i

$$\mathbf{F}_i = \frac{1}{\Delta V_i \Delta t} \sum_{j \in \Delta V_i} \mathbf{n}_j l_j \varepsilon_j$$

- $\mathbf{n}_j$: propagation direction of segment j
- Similarly: K moment includes $n_i n_j$ weighting
- All moments easily obtained by including powers of direction cosines

- Volume-based estimator for J: same packet contributes to multiple cells along its path (not just final cell)
- Demonstrated with homogeneous sphere test — Fig. 12: VBE recovers J, H, K to high accuracy
- Python implementation: update_estimators() routine in mcrt_hom_sphere.py (Appendix B)

9.3.2 Test: Volume-Based Estimators for J, H, K

Fig. 12 — Homogeneous sphere test (Abdikamalov et al. 2012 parameters)

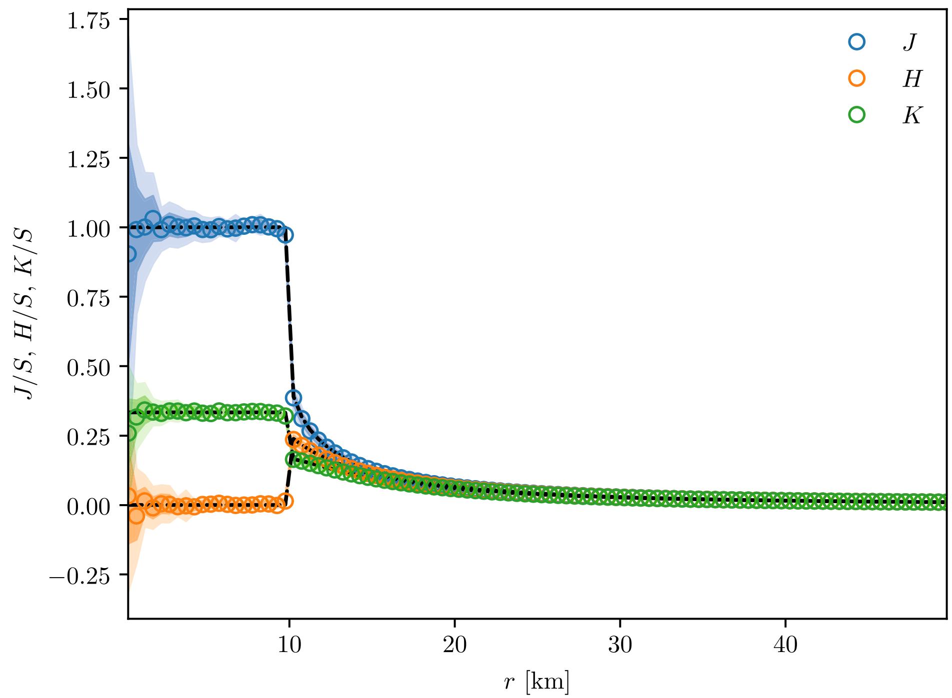

Fig. 12: Volume-based estimators for J (blue), H (orange), K (green) in the homogeneous sphere test. Shown relative to the source function S. Shaded bands: 1σ and 2σ confidence from 10 MCRT runs (10^5 packets each). Open symbols: mean values. Black dashed: analytic solution [Eqs. A.5–A.10]. Agreement is excellent throughout, demonstrating the power of the VBE approach.

9.3.2 Direct Counting vs Volume-Based Estimator

Fig. 13 — Why VBE dramatically outperforms direct counting

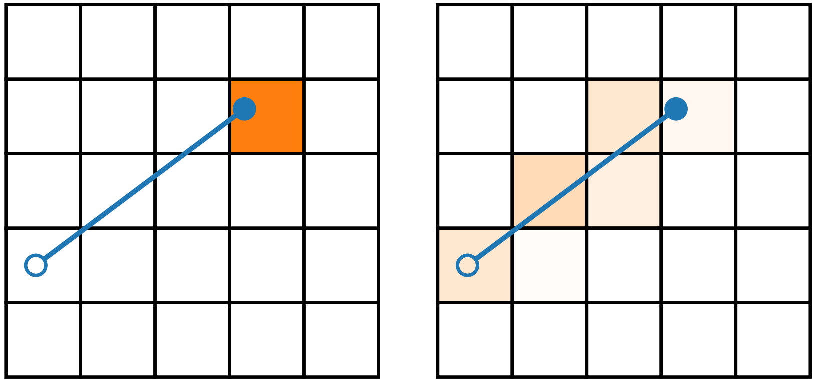

Fig. 13: Single packet trajectory (blue) absorbed at the filled circle. **LEFT (direct counting)**: packet contributes heating rate only in the FINAL cell where absorbed. **RIGHT (volume-based estimator)**: packet contributes to the heating rate estimator in ALL cells it traversed — weighted by the optical depth of each segment. Color transparency encodes the relative contribution to each cell.

Direct Counting Problem

- Only one cell gets information per packet
- All other traversed cells: wasted effort
- Optically thin: rarely absorbed or even none interact → high noise

Volume-Based Estimator Solution

- All traversed cells benefit from trajectory
- Non-zero result even if none absorbed
- Better statistics → lower noise for same N

9.3.3 Constructing VBEs: Extracting Physical Rates

Heating rates, photoionization rates, and momentum deposition

Volume-based approach extends naturally to **physical rates** — not just radiation field moments

- General principle: any rate that depends on the radiation field → substitute VBE for the field
- The optical depth of each segment weights how much interaction the packet COULD have experienced

Heating rate estimator : $\Delta \dot{E} = (1/\Delta V_i c \Delta t) \sum_{j \in \Delta V_i} \chi l_j \varepsilon_j$ $\Leftarrow$ $\text{Normalization}: \quad L = \frac{1}{\Delta t} \sum_{k=1}^{N_{\text{ph}}} \varepsilon_k$

- χ: absorption coefficient (not scattering)
- Gives the total rate of energy absorbed from the radiation field in cell i

Generalization

- Any rate Q proportional to $\chi_\nu J_\nu$ can be estimated:

$$\hat{Q}_i = (1/\Delta V_i c \Delta t) \sum_j \chi_\nu(\nu_j) l_j \varepsilon_j$$

- The sum weights each segment by the appropriate cross-section
- Non-zero as long as ONE packet passed through the cell

Important Note: Line Interactions

- For Sobolev-based line interactions, the formulation is slightly more complicated; they estimators are formed as summations over all packets that have come into resonance within a grid cell (not trajectory segments)
- All resonances contribute even without an actual interaction
- Critical for line-driven wind calculations (Noebauer & Sim 2015)

9.3.4 Example: Photoionization Rate Estimators

A concrete illustration of the VBE principle for atomic rates

- Photoionization rate coefficient $\gamma = 4\pi \int_{\nu_{\rm th}}^{\infty} \frac{\sigma_\nu}{h\nu} J_\nu d\nu$

  Here, σ_ν = photoionization cross section; $\nu_{\rm th}$ = threshold frequency
- Substitute the VBE for J_ν → direct estimator for γ

Photoionization rate estimator : $\hat{\gamma} = (1/\Delta V_i \Delta t) \sum_{j \in \Delta V_i, \nu > \nu_{\rm th}} \frac{\sigma_\nu}{h\nu} l_j \varepsilon_j$

- Sum restricted to segments with $\nu > \nu_{\rm th}$ (photon above threshold)
- Each segment weighted by photoionization cross-section at that frequency

Significance

- Result is non-zero as long as SOME packet above $\nu_{\rm th}$ passed through the cell
- Even one packet gives a statistically useful estimate
- Compare: direct counting requires an actual photoionization event in that cell
- Especially useful in optically thin, highly ionized regions

9.3.5 Energy and Momentum Flow

Similar VBE for radiation flux:

$$F_i = 1/(\Delta V_i c \Delta t) \sum_j n_j l_j \varepsilon_j$$

- Used for radiation momentum deposition in RH calculations
- Particularly important for radiation-driven outflows (Sect. 11)
- Instrument for coupling RT to fluid dynamics

9.4 Biasing — Importance Sampling

Selectively investing computational effort where it matters most

- In many MCRT applications, only a **subset** of packet trajectories contributes to the observable of interest.
- It is therefore desirable to selectively invest more effort into packets that are crucial for the quantity or process of interest instead of treating packets that do not contribute.
- Example: when creating a synthetic image — only packets escaping toward the observer are relevant.

Biasing techniques (known as importance sampling in the MC integration): modify the sampling PDF to over-represent relevant packets

Biasing introduces a new PDF : $q(x) \neq p(x)$. We then sample from this PDF rather than from the physical one $p(x)$.

To maintain physical consistency, the packet weights have to be adjusted:

$$w(x) = \frac{p(x)}{q(x)} w_{\text{nb}} \qquad (w_{\text{nb}} \text{ — weight in the absence of biasing})$$

→ Packets from over-represented regions carry lower weight; under-represented regions carry higher weight.

Key Principle

- Biasing increases statistics where relevant
- Complementary decrease in statistics elsewhere
- Only useful if the 'elsewhere' packets would not contribute anyway
- Widely used in dust RT: Steinacker et al. (2013)

Biasing Techniques Covered (Sect. 9.4)

- 9.4.1 Biased emission
- 9.4.2 Forced scattering
- 9.4.3 Peel-off (next event estimate)
- 9.4.4 Further techniques
- 9.4.5 Russian Roulette & composite biasing

9.4.1 Biased Emission

Over-representing emission from weak or distant sources

- This approach helps in problems where we wish to accurately describe the emission from sources with very different emissivities.
- For instance, consider two sources with very different luminosities $L_1 \ll L_2$.
  - Unbiased: N packets with equal energy $\varepsilon = (L_1 + L_2)\Delta t/N$ — source 1 represented by very few packets
  - Biased: equal number of packets from each source, but with adjusted weights

Unbiased Approach

- Each packet energy: $w = \varepsilon = \dfrac{L\Delta t}{N} \quad (L = L_1 + L_2)$
- Probability of packet from source i : $p_i = L_i/L$
- For $L_1 \ll L_2$: this leads to a very uneven distribution of packets; source 1 represented by ≪ N/2 packets
- High noise for source 1 properties

Biased Approach

- An alternative PDF is introduced that increases the association with the weaker source.
- For instance, use uniform $p_1 = p_2 = 1/2$
- Adjust weights: $w_1 = 2(L_1/L)\varepsilon = 2(L_1\Delta t)/N$
  $w_2 = 2(L_2/L)\varepsilon = 2(L_2\Delta t)/N$
- Both sources equally well-sampled statistically
- Energy conservation maintained via weight adjustment

This approach is also used to preferentially launch packets in **directions of particular interest** (e.g., toward observer)

- Detailed account: Baes et al. (2016) for dust RT applications

9.4.2 Forced Scattering

Two widely-used biasing techniques to improve synthetic observables

Forced Scattering

- Problem: in optically thin media, packets escape without interaction → leading to poor statistics (a low dust-scattering efficiency and challenges in determining heating rates)

- Solution: FORCE at least one interaction before domain edge
  - The interaction location is drawn from the biased PDF, instead of the original PDF $p(\tau)d\tau = \exp(-\tau)d\tau$ for $0 < \tau < \infty$.

$$q(\tau)d\tau = \frac{\exp(-\tau)}{1-\exp(-\tau_{\rm edge})}d\tau \quad \text{if } \tau \le \tau_{\rm edge}$$
$$= 0 \qquad\qquad\qquad\qquad \text{if } \tau > \tau_{\rm edge}$$

  - Weight adjusted:

$$w(\tau) = \frac{p(\tau)}{q(\tau)} = 1 - \exp(-\tau_{\rm edge})$$

- Warning:
  - If continuously applied without an absorption component, this scheme allows packets to propagate indefinitely, with a continuously decreasing weight.continual application → a termination mechanism (e.g., Russian Roulette) has to be introduced to stop the propagation at a certain point, typically once the packet weight has dropped below some pre-defined threshold.
  - **Forced first scattering**: alternatively, **forced scattering can only be applied once** for each packet thus ensuring at least one interaction but leaving the normal propagation termination mechanism (escape through domain edge) intact.

9.4.3 Peel-off

Two widely-used biasing techniques to improve synthetic observables

Peel-off (Next Event Estimate)

- Problem: typically only a small fraction of the packets escapes towards the observer direction.
- Peel-off technique (next event estimate):
  - sometimes referred to as viewpoint technique or virtual packet scheme in the context of MCRT in fast mass outflows.
  - At every interaction point, the probability is calculated that the interaction could have given rise to a packet that propagated in the direction of the observer, and so could contribute to the synthetic observables.

- The weight contributed to the synthetic observables associated with the interaction of a packet with weight w can be written:
  - $w_{\text{obs}} = w \cdot p(\mathbf{n}_{\text{obs}}) \cdot \exp(-\tau_{\text{obs}})$
  - Here, $p(\mathbf{n}_{\text{obs}})$ is the probability that the interaction led to re-emission or scattering of the packet in the direction of the observer ($\mathbf{n}_{\text{obs}}$).
  - $\exp(-\tau_{\text{obs}})$ describes the attenuation of the packet as it travel through the total optical depth from the interaction point to the observer (τ_{obs}). The optical depth is obtained by casting a ray towards the observer and integrating the opacity along this path.
- The peel-off technique can be applied not only to interaction events but instead to all MC packet trajectory elements (Bulla et al. 2015).

Peel-off improvement: every interaction contributes to observer spectrum — not just escaping packets

- Peel-off is particularly powerful for spectral synthesis in SN ejecta and dust RT (Steinacker et al. 2013).
- **Drawback**: ray-tracing to observer adds computational cost significantly, but usually worth it for noise reduction.

9.4.4–9.4.5 Further Biasing Techniques and Limitations

Path length stretching, composite biasing, and Russian Roulette

9.4.4 Further Biasing Techniques

- Path length stretching (Baes et al. 2016)
- Continuous absorption / packet splitting / survival biasing (Carter & Cashwell 1975; Lee et al. 2017)
- Polychromatism (Jonsson 2006; Steinacker et al. 2013)
- See Steinacker et al. (2013) review for comprehensive overview

9.4.5 Limitations of Biasing

- **Drawback**: the increase in statistics in some regions of the parameter space comes at a cost, namely the decrease of statistics in other regions.
  - Biasing techniques should be only used if the loss in statistics happens for packets that are not relevant for the result one is interested in.
- Moreover, **a few high-weight packets may experience an increase in their weight, which in principle is unbound, and thus dominate MC noise.**

Composite biasing — blend biased + original PDF

- To alleviate this deficit of biasing approaches, a technique called composite biasing has been proposed (Baes et al. 2016).
- Samples are drawn from a linear combination of the biased and the original PDF:

$$q^*(x) = (1-\zeta)p(x) + \zeta q(x)$$

Then, the adjusted weight

$$w^* = \frac{p(x)}{q^*(x)} = \frac{1}{(1-\zeta) + \zeta q(x)/p(x)}$$

is limited to $w^* < \frac{1}{1-\zeta}$.

For example, if $\zeta = 1/2$ is chosen, the weight increase can at most be a factor of two.

9.4.4–9.4.5 Further Biasing Techniques and Limitations

Path length stretching, composite biasing, and Russian Roulette

Russian Roulette — Terminating Low-Weight Packets

- When applying biasing techniques that can act multiple times on the same packet, packets with very small weights only contribute insignificantly to the reconstructed property but the same computational efforts has to be investigated to follow their propagation as for important packets.

- It is therefore advisable to terminate the propagation once the weight has decreased beyond some predefined threshold.
- Russian Roulette:
  - Define a termination probability p_T.
  - Whenever a packet enters the roulette (applied once weight drops below a threshold), the termination probability is sampled and the packet propagation is terminated if the sampling outcome is positive. Otherwise, the packet survives and its weight increases to w/p_T.
  - with probability p_T → terminate the packet; with $(1-p_T)$ → survive with weight w/p_T

- Statistically unbiased: surviving packets carry the redistributed weight of terminated ones

- A detailed description and more sophisticated realizations is given by Dupree & Fraley (2002). [A Monte Carlo primer: a practical approach to radiation transport.]

Chapter 9 — Summary

Extracting accurate physical information from MCRT simulations

MC Noise and Estimators

- Fundamental limit: $\sigma \propto N^{-1/2}$
- Direct counting: intuitive but noisy
- Volume-based estimators (Lucy 1999a): use full trajectory, much less noise
- VBE for E, J, H, K, γ, heating rate... all constructable

Biasing Techniques

- Importance sampling: invest effort where it matters
- Biased emission: equal representation of all sources
- Forced scattering: guarantee interactions in thin media
- Peel-off: every interaction contributes to observer
- Russian Roulette: cull low-weight packets safely

- VBE + biasing together allow high-accuracy results with moderate N — essential for practical applications
- These techniques underpin sophisticated codes like ARTIS, SEDONA, TARDIS for SN spectral synthesis
- Next: special MC techniques for **optically thick** regimes (Chapter 10 — IMC and diffusion MC)