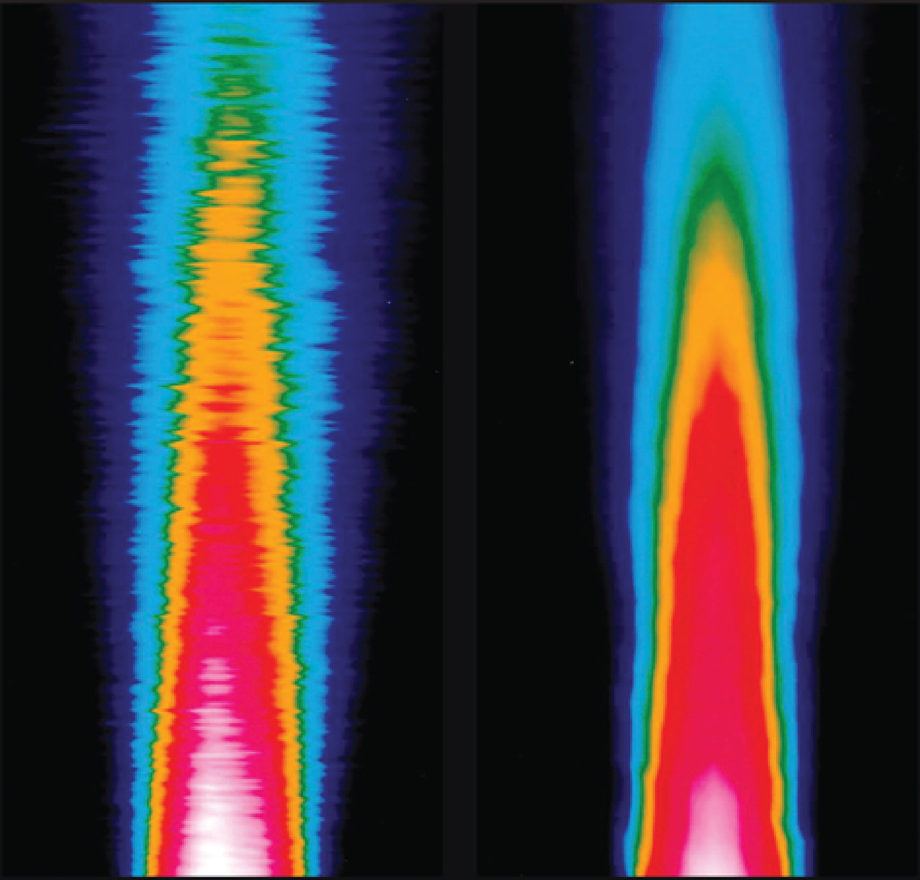

The Monte Carlo Ray-Trace Method in **Radiation Heat Transfer** and Applied Optics

J. Robert Mahan

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THE MONTE CARLO RAY-TRACE METHOD IN RADIATION HEAT TRANSFER AND APPLIED OPTICS

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THE MONTE CARLO RAY-TRACE METHOD IN RADIATION HEAT TRANSFER AND APPLIED OPTICS

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Series Preface

The Wiley-ASME Press Series in Mechanical Engineering brings together two established leaders in mechanical engineering publishing to deliver high-quality, peer-reviewed books covering topics of current interest to engineers and researchers worldwide. The series publishes across the breadth of mechanical engineering, comprising research, design and development, and manufacturing. It includes monographs, references, and course texts. Prospective topics include emerging and advanced technologies in engineering design, computer-aided design, energy conversion and resources, heat transfer, manufacturing and processing, systems and devices, renewable energy, robotics, and biotechnology.

Preface

This book is a stand-alone treatment of the Monte Carlo ray-trace (MCRT) method as it is currently practiced in the field of radiation heat transfer. While intended primarily as a textbook for use by first-year graduate students in curricula such as mechanical and aerospace engineering, the suitability of the MCRT method as an optical modeling tool makes the content equally well suited to the needs of students and practitioners of applied optics.

Max Planck, in his seminal 1912 book **The Theory of Heat Radiation**, writes that when undertaking radiation heat transfer analysis

> *… it will be assumed that the linear dimensions of all parts of space considered, as well as the radii of curvature of all surfaces under consideration, are large compared with the wave lengths of the rays considered. With this assumption we may, without appreciable error, entirely neglect the influence of diffraction caused by the bounding surfaces, and everywhere apply the ordinary laws of reflection and refraction of light.*

In other words, Planck is alerting the reader that radiation heat transfer analysis is to be based on the principles of **geometrical** optics rather than on the more complex principles of **physical** optics. The material presented in the current book extends radiation heat transfer beyond this limited view. By including principles from physical optics we are able to attack problems inaccessible to geometrical optics alone.

During most of the century following the publication of Planck's book, the version of geometrical optics used in radiation heat transfer analysis has been based on its implications rather than on the literal application of its principles. Until the emergence of the high-speed digital computer after World War II, the ray-by-ray application of geometrical optics to complex geometries was simply not practical. By the dawn of the new millennium, however, rapid advances in computing power had made it possible to emit and trace a statistically significant number of rays as they were scattered, refracted, and eventually absorbed within complex enclosures consisting of thousands of surface and optically participating volume elements. In other words, accurate simulation began to displace approximate analysis as a means of describing radiation heat transfer. Today, virtually no serious radiation heat transfer calculations are performed using the antiquated "net exchange" formulation, which is based on the questionable assumptions of uniform surface heat flux and diffuse gray surfaces, and is incapable by itself of treating radiation in participating media.

The mathematical basis of ray tracing and the fundamentals of thermal radiation are presented in the first two chapters. This material prepares the ground for Chapter 3, in which the MCRT method is introduced and used to model radiant exchange among diffuse gray surfaces. After the completion of the first three chapters, the reader is already armed with the essential knowledge required to formulate realistic radiation heat transfer models for the wide range of applications typically encountered in industrial settings. The next three chapters extend the MCRT method to include radiant exchange among non-diffuse non-gray surfaces (Chapter 4), radiation in a participating medium (Chapter 5), and the treatment of polarization, diffraction, and interference in applied optics (Chapter 6). The additional theory required to support these latter topics is introduced as the need arises. The ease of transition from the basic material of Chapter 3 to the more advanced material of Chapters 4, 5, and 6 is remarkable. This is due to the inherent flexibility of the MCRT method itself, whose basic principles apply equally well to directional wavelength-dependent surface models as they do to diffuse gray surface models; and whose logical structure applies equally well to radiant exchange among volume elements as it does to radiant exchange among surface elements. The treatment of polarization, diffraction, and interference using the MCRT method follows naturally after the definition of a "ray" is augmented to include its wavelength, phase, and polarization state. Finally, Chapter 7 presents a formal statistical method for assessing the uncertainty, to a stated level of confidence, of results obtained using the MCRT method.

J. Robert Mahan
Blacksburg
March 2018

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Most of what I know today, and much of the content of this book, I learned through my interaction with the 60 or so outstanding young men and women whose dissertation and thesis research I have had the privilege of directing over a long and rewarding career spent mostly at Virginia Tech. Without the intellectual stimulation they provided, this book simply would not have been possible. Over the years my research has been more or less continuously sponsored by the National Aeronautics and Space Administration, principally by the Climate Science Branch of the Science Directorate at NASA's Langley Research Center. Without this funding, there would have been no graduate students, and thus no book.

I owe an unrepayable debt of gratitude to my own professors at the University of Kentucky, especially to my infinitely patient advisor Clifford J. Cremers, but also to Richard C. Birkebak, John H. Lienhard, IV, and Roger Eichhorn. Their high standards of scholarship, integrity, and achievement have served as a lasting guide for me as I pursued my own academic career.

Finally, my wife, Bea, who has been my constant companion for more than 50 years, has made the voyage worthwhile.

J. Robert Mahan
Blacksburg

About the Companion Website

This book is accompanied by a companion website:

www.wiley.com/go/mahan/monte-carlo

There is a website for Instructor and Students separately. The Website includes:

1) Solution manual
2) Data Tables
3) Analytical tools
4) Matlab codes

Scan this QR code to visit the companion website.

1

Fundamentals of Ray Tracing

A ray is defined as the collection of straight-line path segments followed by an energy bundle from its point of emission to its point of absorption. The definition includes the possibility of intermediate reflection, scattering, refraction, and even diffraction events. Ray tracing involves the application of basic mathematics to the process of identifying the intersection of ray segments with surfaces. Most engineering and science students acquire the required mathematical tools long before they enter university. The current chapter provides a review of the mathematical principles governing ray tracing and the related issues of meshing and indexing.

1.1 Rays and Ray Segments

A **ray** is defined here as the continuous sequence of straight-line paths connecting a point on one surface, from which an energy bundle is emitted, to a point on a second surface – or perhaps even on the same surface – where it is ultimately absorbed. One or several reflections from intervening surfaces may occur between emission and absorption of the energy bundle. The path followed by the energy bundle between

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reflections is referred to as a **ray segment**. Two situations are normally considered: either (i) the power of the emitted energy bundle does not change as it is reflected from one surface to the next until it reaches the surface where all its power is ultimately absorbed; or (ii) a fraction of the emitted power is left behind with each reflection until the remaining power is deemed to have dropped below a threshold value, at which point the ray trace is terminated. Both approaches have their adherents and are in common use, and both are developed in detail in this book.

1.2 The Enclosure

The **enclosure** is an essential concept in all approaches to radiation heat transfer analysis. We define the enclosure as an ensemble of surfaces, both real and imaginary, arranged in such a manner that a ray emitted into the interior of the enclosure cannot escape. Energy is conserved within the enclosure under this definition. If a ray does leave the enclosure through an opening, represented by an imaginary surface, the energy it carries is deducted from the overall energy balance.

1.3 Mathematical Preliminaries

Consider two points, P_0 and P_1, in three-dimensional space, as illustrated in Figure 1.1. Let the Cartesian coordinates of points P_0 and P_1 be (x_0, y_0, z_0) and (x_1, y_1, z_1), respectively. Then the vector directed from P_0 to P_1 is

$$\boldsymbol{V} = (x_1 - x_0)\,\boldsymbol{i} + (y_1 - y_0)\boldsymbol{j} + (z_1 - z_0)\,\boldsymbol{k}, \tag{1.1}$$

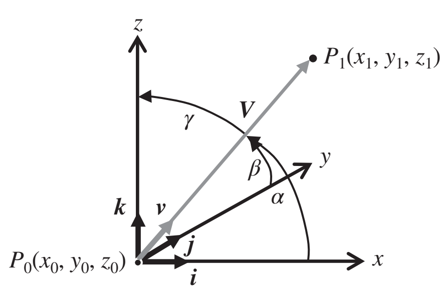

Figure 1.1 Relationships among the quantities introduced in Section 1.3.

and its magnitude is

$$t \equiv \sqrt{|\boldsymbol{V} \cdot \boldsymbol{V}|} = \sqrt{(x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2}. \tag{1.2}$$

In Eq. (1.1) $\boldsymbol{i}, \boldsymbol{j}$, and $\boldsymbol{k}$ are the unit vectors directed along the x-, y-, and z-axes, respectively. Note that the distance t from P_0 to P_1 must always be real and positive.

The unit vector in the direction of $\boldsymbol{V}$ is

$$\boldsymbol{v} \equiv \boldsymbol{V}/t = L\,\boldsymbol{i} + M\boldsymbol{j} + N\,\boldsymbol{k}, \tag{1.3}$$

where L, M, and N are the **direction cosines** illustrated in Figure 1.1. The direction cosines are defined

$$L \equiv \boldsymbol{v} \cdot \boldsymbol{i} = \cos\alpha, M \equiv \boldsymbol{v} \cdot \boldsymbol{j} = \cos\beta, \text{and } N \equiv \boldsymbol{v} \cdot \boldsymbol{k} = \cos\gamma, \tag{1.4}$$

where α, β, and γ are the angles between the unit vector $\boldsymbol{v}$ and the x-, y-, and z-axes, respectively. Equations (1.1) and (1.3) can be combined to define the equations for the line segment connecting point P_0 to point P_1

$$(x_1 - x_0)/L = (y_1 - y_0)/M = (z_1 - z_0)/N = t. \tag{1.5}$$

The three equations embodied in Eq. (1.5) are arguably the most important relationships in geometrical optics, because they form the basis for navigation of rays within an enclosure.

The general equation for a **surface** in Cartesian coordinates is

$$S(x, y, z) = 0. \tag{1.6}$$

The simplest, and perhaps most common, surface used in fabricating an enclosure is the plane, illustrated in Figure 1.2. In order to derive the equation for a plane, we must know the unit normal vector $\boldsymbol{n}$ at a point

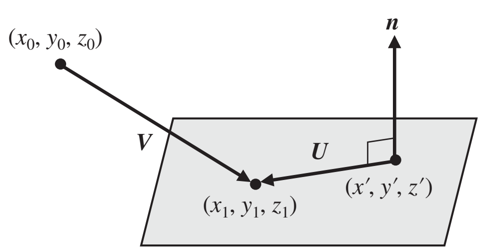

Figure 1.2 Definition of a plane surface.

(x', y', z') in the plane and the coordinates of a second point (x_1, y_1, z_1) in the plane. Then, because $\boldsymbol{n}$ and $\boldsymbol{U}$ are in quadrature, it must be true that

$$\begin{aligned} S(x_1, y_1, z_1) &= \boldsymbol{n} \cdot \boldsymbol{U} \\ &= \boldsymbol{n} \cdot [(x_1 - x')\,\boldsymbol{i} + (y_1 - y')\,\boldsymbol{j} + (z_1 - z')\,\boldsymbol{k}] \\ &= 0, \end{aligned} \tag{1.7}$$

or

$$S(x_1, y_1, z_1) = n_x\,(x_1 - x') + n_y\,(y_1 - y') + n_z\,(z_1 - z') = 0. \tag{1.8}$$

To find the intersection of the ray segment $\boldsymbol{V} = (x_1 - x_0)\,\boldsymbol{i} + (y_1 - y_0)\,\boldsymbol{j} + (z_1 - z_0)\,\boldsymbol{k}$ with the plane, we introduce Eq. (1.5) into Eq. (1.8), obtaining

$$n_x\,(x_0 + Lt - x') + n_y\,(y_0 + Mt - y') + n_z\,(z_0 + Nt - z') = 0. \tag{1.9}$$

Finally, solving Eq. (1.9) for t we obtain

$$t = \frac{n_x(x' - x_0) + n_y(y' - y_0) + n_z(z' - z_0)}{n_x L + n_y M + n_z N}, \tag{1.10}$$

or

$$t = \frac{\boldsymbol{n} \cdot (\boldsymbol{V} - \boldsymbol{U})}{\boldsymbol{n} \cdot \boldsymbol{v}}. \tag{1.11}$$

Note that if $\boldsymbol{n}$ and **v** are in quadrature, $\boldsymbol{n} \cdot \boldsymbol{v} = 0$, in which case t is undefined. The interpretation is that the ray passes parallel to the plane and so can never intersect it. We must anticipate this eventuality when programming. This is perhaps an appropriate juncture to emphasize the natural compatibility of Cartesian coordinates with the vector nature of ray tracing.

A more instructive example is the intersection of a ray segment with a sphere of radius R whose center is located at (x_C, y_C, z_C); that is,

$$S(x_1, y_1, z_1) = (x_1 - x_C)^2 + (y_1 - y_C)^2 + (z_1 - z_C)^2 – R^2 = 0. \tag{1.12}$$

Suppose a ray is emitted from point (x_0, y_0, z_0) in the direction (L, M, N) and we want to find its point of intersection (x_1, y_1, z_1) with this sphere. As in the previous example, this may be accomplished by finding the point (x_1, y_1, z_1) that simultaneously satisfies the three equations for the straight line connecting the two points, Eq. (1.5), and the equation for the sphere, Eq. (1.12); that is,

$$(x_0 + Lt - x_C)^2 + (y_0 + Mt - y_C)^2 + (z_0 + Nt - z_C)^2 - R^2 = 0. \tag{1.13}$$

Happily, the solution of Eq. (1.13) for the distance t is just about the most challenging mathematical operation we encounter in ray tracing.

It is convenient to use the symbolic solver feature of Matlab to solve quadratic equations (see Problems 1.2–1.7). However, solution of Eq. (1.13) is relatively straightforward and provides an opportunity to point out certain useful properties of the quadratic coefficients. Upon carrying out the indicated operations and rearranging the result, we have

$$(L^2 + M^2 + N^2)\, t^2 + 2[L(x_0 - x_C) + M(y_0 - y_C) + N(z_0 - z_C)]\, t + (x_0 - x_C)^2 + (y_0 - y_C)^2 + (z_0 - z_C)^2 - R^2 = 0, \tag{1.14}$$

or

$$A\, t^2 + B\, t + C = 0, \tag{1.15}$$

where

$$A = L^2 + M^2 + N^2, \tag{1.16}$$

$$B = 2[L(x_0 - x_C) + M(y_0 - y_C) + N(z_0 - z_C)], \tag{1.17}$$

and

$$C = (x_0 - x_C)^2 + (y_0 - y_C)^2 + (z_0 - z_C)^2 - R^2. \tag{1.18}$$

The coefficients A, B, and C are defined in terms of known quantities and, thus, are themselves known. Equation (1.14) can now be solved for t, yielding

$$t_1 = (-B + \sqrt{B^2 - 4AC})/2A \text{ and } t_2 = (-B - \sqrt{B^2 - 4AC})/2A. \tag{1.19}$$

We define a **quadratic surface** as any surface whose algebraic equation $S(x, y, z) = 0$ is second-order. It turns out that, in addition to plane surfaces, essentially all enclosures of practical engineering interest include such surfaces or surfaces that can be subdivided into such surfaces. Listed in Table 1.1 are some of the quadratic surfaces commonly encountered in radiation heat transfer and applied optics. Equation (1.19), with generally different expressions for the coefficients A, B, and C, yields the candidate values of the distance t for all quadratic surfaces.

Note that Eq. (1.19) has two roots, t_1 and t_2. The physical interpretation of two roots is that a given ray "intersects" the spherical surface at two points. However, the intersection may be **degenerate** (both roots corresponding to the same point) or **imaginary** (the ray does not physically intersect the sphere). Only in the case of plane surfaces are single,

Table 1.1 Quadratic surfaces commonly encountered in radiation heat transfer and applied optics modeling.

Name	$S(x, y, z) = 0$	Notes
Sphere	$(x - x_C)^2 + (y - y_C)^2 + (z - z_C)^2 - R^2 = 0$	R = radius, center at (x_C, y_C, z_C)
Tri-axial ellipsoid	$\frac{(x - x_C)^2}{a^2} + \frac{(y - y_C)^2}{b^2} + \frac{(z - z_C)^2}{c^2} - 1 = 0$	a, b, c = semi-axes, center at (x_C, y_C, z_C)
Spheroid	$\frac{(\mathrm{x} - \mathrm{x_C})^2}{\mathrm{a}^2} + \frac{(\mathrm{y} - \mathrm{y_C})^2}{\mathrm{a}^2} + \frac{(\mathrm{z} - \mathrm{z_C})^2}{\mathrm{c}^2} - 1 = 0$	Prolate if $c > a$, oblate if $c < a$, center at (x_C, y_C, z_C)
Elliptic paraboloid	$\frac{(\mathrm{x} - \mathrm{x_C})^2}{\mathrm{a}^2} + \frac{(\mathrm{y} - \mathrm{y_C})^2}{\mathrm{b}^2} - \mathrm{z} = 0$	Upward-opening, origin at $(\mathrm{x_C}, \mathrm{y_C}, \mathrm{z_C})$
Hyperbolic paraboloid ("Potato chip")	$(x/a)^2 - (y/b)^2 - z = 0$	Opens up along x-axis, down along y-axis
Two-sheet hyperboloid	$(x/a)^2 + (y/a)^2 - (z/c)^2 + 1 = 0$	Rotationally symmetric about z-axis
Right-circular cone	$(x - x_v)^2 + (y - y_v)^2 - tan^2\alpha\,(z - z_v)^2 = 0$	Vertex at (x_v, y_v, z_v), α = cone half-angle
Right-circular cylinder	$x^2 + y^2 - R^2 = 0,\ 0 \le z \le h$	Rotationally symmetric about z-axis, h = height

non-degenerate roots obtained. More than two roots arise in the case of higher-order surfaces but, as has already been pointed out, most enclosures of practical engineering interest are composed of either planes or quadratic surfaces.

The physical significance of quadratic roots is illustrated in Figure 1.3. If both roots are real ($B^2 > 4AC$) in Eq. (1.19), the ray emitted from P_0 intersects the surface at two points, P_1 and P_2, where one corresponds to the plus (+) sign in Eq. (1.19) and the other corresponds to the minus (−) sign. If $B^2 = 4AC$, the roots are degenerate and the single solution, $t = -B/2A$, is obtained. This signifies that the ray is tangent to the sphere at a single point P_3. Finally, if both roots are complex ($B^2 < 4AC$), the ray fails to intersect the surface.

At the most, only one real root is physically significant. How do we choose between the two available real roots? This is a trivial choice for someone provided with an image such as Figure 1.3; however, a computer requires an algorithm based on the values of the quadratic coefficients A, B, and C. In the special case of a sphere we recognize that $A = \sqrt{\boldsymbol{v} \cdot \boldsymbol{v}} = 1$, where the vector $\boldsymbol{v}$ is given by Eq. (1.3). While this simplifies the algebra somewhat, it does not otherwise contribute to the process of identifying the correct root. The coefficient B in the case of a sphere can be expressed

$$B/2 = \boldsymbol{v} \cdot \boldsymbol{V}_0, \tag{1.20}$$

where $\boldsymbol{V_0}$ is the vector directed from the center of the sphere (x_C, y_C, z_C) to the source point (x_0, y_0, z_0),

$$\boldsymbol{V}_0 = (x_0 - x_C)\,\boldsymbol{i} + (y_0 - y_C)\boldsymbol{j} + (z_0 - z_C)\,\boldsymbol{k}. \tag{1.21}$$

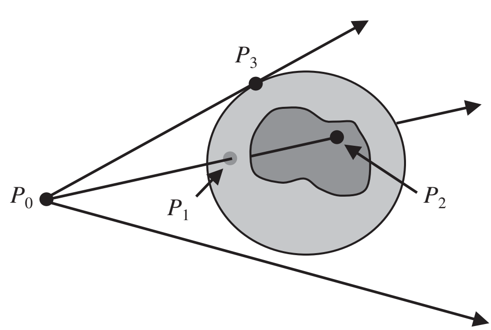

Figure 1.3 Possible disposition of three rays emitted from point P_0.