# Ray Optics Module

## User's Guide

COMSOL

# Ray Optics Module User's Guide

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# Chapter 1: Introduction

# Chapter 2: Ray Optics Modeling

# Chapter 3: Ray Optics Interfaces

# Chapter 4: Multiphysics Interfaces and Couplings

# Chapter 5: Glossary

# 1

# Introduction

This guide describes the Ray Optics Module, an optional add-on package for COMSOL Multiphysics®.

This chapter introduces you to the capabilities of this module. A summary of the physics interfaces and where you can find documentation and model examples is also included. The last section is a brief overview with links to each chapter in this guide.

In this chapter:

- About the Ray Optics Module
- Overview of the User's Guide

# About the Ray Optics Module

These topics are included in this section:

- The Ray Optics Module Physics Interface Guide
- Common Physics Interface and Feature Settings and Nodes
- Where Do I Access the Documentation and Application Libraries?

## *The Ray Optics Module Physics Interface Guide*

The Ray Optics Module extends the functionality of the physics interfaces in COMSOL Multiphysics with physics interfaces for geometrical optics and ray heating, where the rays can be polarized, unpolarized, or partially polarized. There are also tools for computing the intensity, phase, and optical path length of rays. The details of the physics interfaces and study types for the Ray Optics Module are listed in the table below. The functionality of the COMSOL Multiphysics base package is given in the *COMSOL Multiphysics Reference Manual*.

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| | |
|---|---|
| 🔍 | In the *COMSOL Multiphysics Reference Manual*:<br><br>- Studies and Solvers<br>- The Physics Interfaces<br>- For a list of all the core physics interfaces included with a COMSOL Multiphysics license, see Physics Interface Guide. |

| PHYSICS INTERFACE | ICON | TAG | SPACE DIMENSION | AVAILABLE STUDY TYPE |
|---|---|---|---|---|
| ⫴ᐳ **Optics** | | | | |
| ⟋ᐳᴸ **Ray Optics** | | | | |
| Geometrical Optics | ◖ᐳ | gop | 3D, 2D, 2D axisymmetric | ray tracing; bidirectionally coupled ray tracing; time dependent |
| Ray Heating | ⟋ᐳᴸ | — | 3D, 2D, 2D axisymmetric | ray tracing; bidirectionally coupled ray tracing; time dependent |

## Common Physics Interface and Feature Settings and Nodes

There are several common settings and sections available for the physics interfaces and feature nodes. Some of these sections also have similar settings or are implemented in the same way no matter the physics interface or feature being used. There are also some physics feature nodes that display in COMSOL Multiphysics.

In each module's documentation, only unique or extra information is included; standard information and procedures are centralized in the *COMSOL Multiphysics Reference Manual*.

> ⚠ In the *COMSOL Multiphysics Reference Manual* see Table 2-4 for links to common sections and Table 2-5 to common feature nodes. You can also search for information: press F1 to open the **Help** window or Ctrl+F1 to open the **Documentation** window.

## Where Do I Access the Documentation and Application Libraries?

A number of online resources have more information about COMSOL, including licensing and technical information. The electronic documentation, topic-based (or

context-based) help, and the Application Libraries are all accessed through the COMSOL Desktop.

> ⚠️ If you are reading the documentation as a PDF file on your computer, the blue links do not work to open an application or content referenced in a different guide. However, if you are using the Help system in COMSOL Multiphysics, these links work to open other modules, application examples, and documentation sets.

### THE DOCUMENTATION AND ONLINE HELP

The *COMSOL Multiphysics Reference Manual* describes the core physics interfaces and functionality included with the COMSOL Multiphysics license. This book also has instructions on how to use COMSOL Multiphysics and how to access the electronic Documentation and Help content.

*Opening Topic-Based Help*

The Help window is useful as it is connected to the features in the COMSOL Desktop. To learn more about a node in the Model Builder, or a window on the Desktop, click to highlight a node or window, then press F1 to open the Help window, which then displays information about that feature (or click a node in the Model Builder followed by the **Help** button ( ? ). This is called *topic-based* (or *context) help*.

> **Win**
>
> To open the **Help** window:
>
> - In the **Model Builder**, **Application Builder**, or **Physics Builder**, click a node or window and then press F1.
> - On any toolbar (for example, **Home**, **Definitions**, or **Geometry**), hover the mouse over a button (for example, **Add Physics** or **Build All**) and then press F1.
> - From the **File** menu, click **Help** ( ? ).
> - In the upper-right corner of the COMSOL Desktop, click the **Help** ( ? ) button.

To open the **Help** window:

- In the **Model Builder** or **Physics Builder**, click a node or window and then press F1.
- On the main toolbar, click the **Help** ( ? ) button.
- From the main menu, select **Help>Help**.

Mac

Linux

*Opening the Documentation Window*

To open the **Documentation** window:

Win

- Press Ctrl+F1.
- From the **File** menu, select **Help>Documentation** ( ▉ ).

To open the **Documentation** window:

Mac

- Press Ctrl+F1.
- On the main toolbar, click the **Documentation** ( ▉ ) button.

Linux

- From the main menu, select **Help>Documentation**.

### THE APPLICATION LIBRARIES WINDOW

Each model or application includes documentation with the theoretical background and step-by-step instructions to create a model or application. The models and applications are available in COMSOL Multiphysics as MPH-files that you can open for further investigation. You can use the step-by-step instructions and the actual models as templates for your own modeling. In most models, SI units are used to describe the relevant properties, parameters, and dimensions, but other unit systems are available.

Once the Application Libraries window is opened, you can search by name or browse under a module folder name. Click to view a summary of the model or application and its properties, including options to open it or its associated PDF document.

The Application Libraries Window in the *COMSOL Multiphysics Reference Manual*.

*Opening the Application Libraries Window*
To open the **Application Libraries** window ( ▯▯▯ ):

| | |
|---|---|
| Win | From the **File** menu, select **Application Libraries**.<br><br>To include the latest versions of model examples, from the **File>Help** menu, select ( 🔲 ) **Update COMSOL Application Library**. |

| | |
|---|---|
| Mac<br><br>Linux | Select **Application Libraries** from the main **File** or **Windows** menus.<br><br>To include the latest versions of model examples, from the **Help** menu, select ( 🔲 ) **Update COMSOL Application Library**. |

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**COMSOL ONLINE RESOURCES**

| | |
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| Events | www.comsol.com/events |
| COMSOL Application Gallery | www.comsol.com/models |
| COMSOL Video Gallery | www.comsol.com/video |
| Support Knowledge Base | www.comsol.com/support/knowledgebase |

# Overview of the User's Guide

The *Ray Optics Module User's Guide* gets you started with modeling using COMSOL Multiphysics. The information in this guide is specific to this module. Instructions how to use COMSOL in general are included with the *COMSOL Multiphysics Reference Manual*.

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As detailed in the section Where Do I Access the Documentation and Application Libraries? this information can also be searched from the COMSOL Multiphysics software **Help** menu.

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### TABLE OF CONTENTS AND INDEX

To help you navigate through this guide, see the Contents and Index.

### RAY OPTICS MODELING

The Ray Optics Modeling chapter provides an overview of ray tracing simulation. It begins with an overview of the Essentials of Ray Tracing. It then describes the major functionality groups that are included in The Geometrical Optics Interface, including topics such as Geometry and Meshing, Ray Release Features, Study Types, and Results Analysis and Visualization.

### RAY OPTICS INTERFACES

The Ray Optics Interfaces chapter describes The Geometrical Optics Interface and includes the Theory for the Geometrical Optics Interface.

### MULTIPHYSICS INTERFACES AND COUPLINGS

The Multiphysics Interfaces and Couplings chapter describes The Ray Heating Interface, a dedicated multiphysics interface for computing heat sources generated by attenuation of rays in absorbing media, and includes the Theory for the Ray Heating Interface.

# 2

# Ray Optics Modeling

This chapter gives an overview of the most important considerations when creating a ray optics model. The most significant modeling decisions include the means of geometry setup, the choice of optical material properties, ray releases, and handling of ray interactions with surfaces in the geometry.

In this chapter:

- Essentials of Ray Tracing
- Geometry and Meshing
- Domain Properties
- Boundary Conditions
- Ray Release Features
- Additional Variables Solved For
- Study Types
- Results Analysis and Visualization
- Variables and Nonlocal Couplings
- Material Libraries

# Essentials of Ray Tracing

The Geometrical Optics interface can be used to simulate cameras, telescopes, laser and illumination systems, spectrometers, solar collectors, and much more. However, certain essential elements of the ray optics approach are common to all of these application areas. These universal concepts in ray optics simulation are outlined below.

In this section:

- The Ray Tracing Algorithm
- Basic Requirements of a Geometrical Optics Model

## The Ray Tracing Algorithm

The Geometrical Optics interface solves for the position and wave vector of individual rays. It also allows them to interact with boundaries that intersect their paths.

Ray tracing is usually a reasonable approach to modeling electromagnetic wave propagation if the wavelength of the radiation is small compared to the smallest geometric detail in the surroundings, since diffraction is ignored. As long as this criterion is met, ray tracing can be used for nearly any part of the electromagnetic spectrum, including radio waves, microwaves, visible light, and UV radiation. Note that X-ray modeling may require the consideration of diffraction effects because X-rays can interact with matter on an atomic level.

If the geometry is on the wavelength scale, you might also consider a multiscale approach by first solving for the electric field in the frequency domain using the finite element method (FEM) and then using the FEM solution to define a ray release.

While propagating through a homogeneous medium (one in which the refractive index is spatially uniform), a ray simply goes in a straight line at speed $c/n$, where $c = 299,792,458$ m/s is the speed of light in a vacuum and $n$ (dimensionless) is the absolute refractive index of the medium. In a graded-index medium, the ray can follow a curved path, which is determined by integrating coupled first-order ordinary differential equations over time.

> To learn more about the equations of ray propagation and their derivation, see Introduction to Geometrical Optics in the Theory for the Geometrical Optics Interface chapter.

The Geometrical Optics interface is compatible with the **Ray Tracing**, **Time Dependent**, and **Bidirectionally Coupled Ray Tracing** study steps. These study types are very similar, except that the **Ray Tracing** study step makes it possible to specify either a list of optical path length intervals or a list of time steps. (Internally, the optical path lengths are converted to the corresponding times, so this is just a matter of convenience.)

For simple ray tracing models, only the first and last path lengths or time steps might be needed. The behavior of rays at any intermediate time can then be accurately interpolated. If rays interact with boundaries in between the stored time steps, then the exact time and position of each ray-boundary interaction is also stored and readily available.

Finer stepping in time or path length may be needed when modeling ray propagation in graded-index media, when rays pass through attenuating media and generate heat in their surroundings, or when using specialized postprocessing features.

Every time the intersection of a ray with a surface is detected, a wide variety of ray-boundary interactions may apply. These include specular reflection, diffuse reflection, refraction, and several different types of absorption.

Along each ray, it is possible to evaluate expressions that involve variables defined on the ray itself (such as optical path length, intensity, and wavelength) and variables defined at the ray's position in the modeling domain (such as temperature and refractive index). For example, to determine the refractive index in an optically dispersive medium, an expression is evaluated on each ray that combines the ray's wavelength or frequency with a function queried from the domain the ray occupies. Similarly, when a ray hits a boundary, the new direction of the ray can depend on a combination of ray variables (like wavelength) and surface variables (like surface normal direction and Gaussian curvature).

## Basic Requirements of a Geometrical Optics Model

Although geometrical optics models vary tremendously in application area and scope, every geometrical optics model requires at least the following basic features:

- A geometry must be present, with at least one surface that can interact with the rays.
- The refractive index must be specified. If any domains are present, use the Medium Properties node to either specify the refractive index directly or specify which material controls it.
- The model must have at least one *boundary condition*, such as the Material Discontinuity or Wall node. By default, every boundary adjacent to at least one

domain in the model is treated as a **Material Discontinuity** that can reflect and refract rays. See Boundary Conditions for more information.

- Every model includes the Ray Properties node, a default node that cannot be removed. This node defines the equations of ray propagation. If the radiation is monochromatic, this is also where you specify the frequency or wavelength.

- Some rays must be released into the model. This requires at least one r*ay release feature,* such as the Release, Release from Boundary, or Release from Grid node. See Ray Release Features for more details.

- The ray tracing algorithm detects ray-boundary interactions using the underlying finite element mesh. At the very least, a surface mesh is needed. For multiphysics modeling in which field variables like temperature are solved for, a domain mesh is also necessary. Some related topics are discussed in the Geometry and Meshing. section.

- A study is necessary to compute the ray paths. The Geometrical Optics interface is compatible with the **Time Dependent**, **Ray Tracing**, and **Bidirectionally Coupled Ray Tracing** study steps. **Ray Tracing** is recommended for most models. See Study Types for more information.
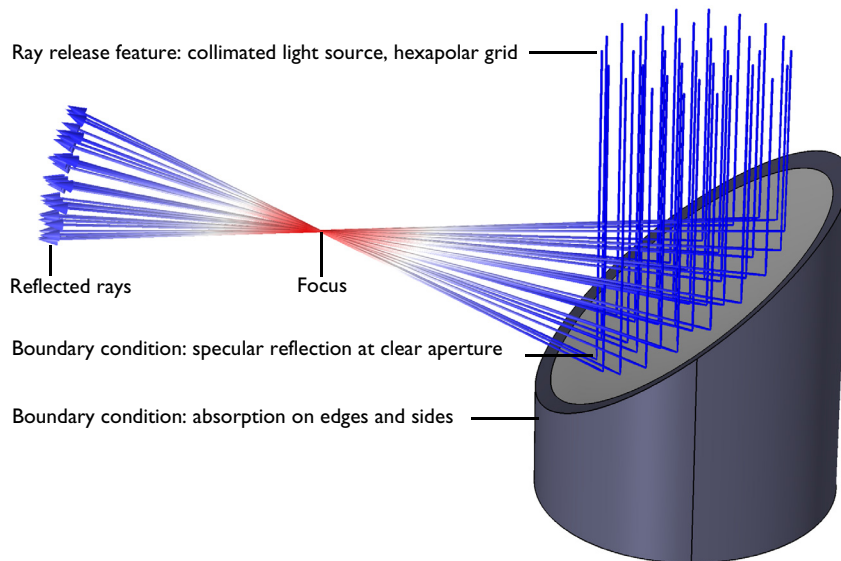


*Figure 2-1: A simple ray tracing model, featuring specular reflection of a collimated beam by an off-axis conic mirror. The color expression indicates the ray intensity.*

# Geometry and Meshing

Electromagnetic radiation can interact with a wide variety of geometric entities. In ray optics simulation, the most common elements include lenses, mirrors, prisms, beam splitters, light pipes, and various obstructions. Rays may also interact with buildings, vehicles, people, planets, and more.

In this section, various considerations for setting up the model geometry and the associated finite element mesh are considered in more detail:

- Creating a Geometry
- Domain Selection
- Meshing and Discretization Error
- Meshing Guidelines

## *Creating a Geometry*

The Geometrical Optics interface supports interaction with any geometric entity. The geometry can be constructed from built-in primitives like circles and line segments, loaded from various CAD formats, or constructed with parts from the Ray Optics Part Library. Rays can interact with both deformed and undeformed geometries, for example, when an object undergoes thermal expansion.

### PART LIBRARIES

In ray optics models, it is often necessary to set up geometry sequences consisting of entities that are more complex than simple geometry primitives such as spheres, cones, and blocks. Instead it might be necessary to insert lenses with different thicknesses and radii of curvature, off-axis conic mirrors, and parabolic concentrators. The entity shapes might need to be resolved to extremely high precision. This can be conveniently accomplished using the Part Libraries for the Ray Optics Module.

The Ray Optics Module Part Libraries contain fully parameterized sequences of geometry instructions that produce more complex shapes frequently required for geometrical optics simulation, including the following:

- Spherical lenses and mirrors
- Conic lenses and mirrors
- Aspheric lenses and mirrors (even, odd, and Q-type)

- Doublet and triplet lenses
- Cylindrical lenses
- Beam splitters
- Polygonal mirrors
- Prisms
- Circular and rectangular annuli
- Retroreflectors

For example, you can load the *Spherical Lens 3D* part into a model and then specify the radii of curvature of each lens surface, along with the lens thickness and diameter.

Parts can include predefined selections that make it easy to apply boundary conditions or material properties to multiple geometric entities at the same time. Some parts also include multiple variants or different sets of inputs that you can choose between. For example, you could either specify the off axis distance or off axis angle for a conic mirror.

In addition, many parts automatically define work planes so that the parts and other features can more easily be positioned and oriented with respect to each other.

| | Many Ray Optics tutorials use the Part Library to create their geometry sequences. To learn more, see the following models: <br><br> • *Newtonian Telescope*: Application Library path **Ray_Optics_Module/ Lenses_Cameras_and_Telescopes/newtonian_telescope** <br><br> • *Petzval Lens*: Application Library path **Ray_Optics_Module/ Lenses_Cameras_and_Telescopes/petzval_lens** |
|---|---|

| | Part Libraries in the *COMSOL Multiphysics Reference Manual*. |
|---|---|

### RAY TRACING IN AN IMPORTED MESH

It is possible to compute ray trajectories in an imported mesh. The mesh can be imported from a COMSOL Multiphysics file (.mphbin for a binary file format or .mphtxt for a text file format) or from a NASTRAN file (.nas, .bdf, .nastran, or .dat).

If the mesh is imported from a COMSOL Multiphysics file, the imported mesh always uses a linear geometry shape order for the purpose of modeling ray-boundary interactions, even if the model used to generate the mesh had a higher geometry shape order.

If the mesh is imported from a NASTRAN file, the ray-boundary interactions can be modeled using either a linear or higher geometry shape order. If **Export as linear elements** is selected when generating the NASTRAN file, or if **Import as linear elements** is selected when importing the file, then linear geometry shape order will be used.

### Domain Selection

It is possible for rays to pass through domains in the geometry and to propagate in the void region outside these domains. Boundary conditions can be specified at any boundary, including boundaries that are not adjacent to any domain in the geometry. This means that rays can be reflected or absorbed by a surface in 3D, or a line segment in 2D, even if it is not attached to any other object. The ray tracing algorithm can also detect boundary interactions in any order, without this order being specified.

Usually, the domain selection for the Geometrical Optics interface should include all objects that the rays might pass through. In a lens system, this would mean that all lenses are included but not necessarily the mount for these lenses.

Domains that are not included in the selection for the physics interface do not need to be meshed. However, these domains would still require a mesh if some other variables, like displacement and temperature, are solved for there. See Meshing Guidelines for more details.

> Some physics features require a domain mesh and will not function on domains outside the physics interface selection. This includes all types of Accumulator (Domain) feature, such as the dedicated Ray Heat Source multiphysics feature.

### Meshing and Discretization Error

In the Geometrical Optics interface, rays interact with a surface when they hit a mesh element in that surface's boundary mesh. When rays need information about the surface they hit, such as the surface normal direction, which controls the direction of

reflected and refracted rays, this information is also evaluated on the boundary mesh. Thus, having a high-quality mesh is an integral part of ray optics simulation.

The use of a boundary mesh to detect and apply ray-boundary interactions makes the Geometrical Optics interface readily extensible to high-fidelity multiphysics simulation, including such effects as translational motion, rotation, and structural deformation of the geometry (including thermal stress). In addition, this implementation makes it possible to trace rays through geometric entities of arbitrary shape, not just simple shapes for which a parametric representation is readily available.

Because rays interact with a mesh representation of the geometry, the mesh must be adequately refined so that the coordinates of points along the surface are sufficiently accurate. The level of mesh refinement also affects the accuracy of the tangential and normal unit vectors that are defined on the boundary elements, as well as the Gaussian curvatures that may be used to calculate the intensity along rays. Very high accuracy can be achieved with a coarse mesh on planar surfaces because even a small number of linear boundary elements can represent a planar surface to machine precision. Accurately discretizing the geometry becomes more important when the surfaces are curved, as in spherical lenses and conic mirrors, or when the surfaces can be deformed.

In the following image, the radial position over one boundary element on a coarsely meshed sphere (using quadratic elements) is compared to the exact value for an ideal sphere. The error is on the order of $10^{-5}$.
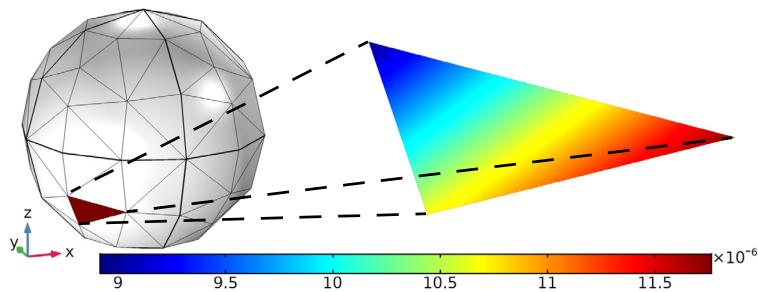


*Figure 2-2: Error in the radial displacement over one boundary element of a unit sphere.*

A relative error like the one shown above ($10^{-5}$) might be sufficiently small for some simulation results, but in geometrical optics such an error might translate to tens of additional wavelengths in spot size — large enough to invalidate the results of the simulation entirely, unless adequate precautions are taken. Similarly, in models with

mesh deformation, the degrees of freedom for the displacement field must be solved for extremely accurately for the results of a coupled multiphysics model to be trusted. A good practice, as with other types of simulation, is to perform a mesh refinement study, ensuring that the results do not change appreciably when the mesh element size is reduced further.

Note that ray tracing in COMSOL uses double precision floating point arithmetic, in for which machine precision is of order $10^{-16}$.

## *Meshing Guidelines*

- Flat edges (2D) and planar surfaces (3D) can be coarsely meshed, unless they meet one of the criteria described below.

- Curved surfaces that can interact with rays should always be finely meshed. The tighter the curvature of such surfaces, the finer the mesh should be.

- In 3D, the row of curved boundary elements adjacent to a curved edge are more susceptible to mesh discretization error than boundary elements that are not adjacent to an edge. For this reason, avoid unnecessary interior edges in 3D.

- Domains usually do not need to be as finely meshed as boundaries. A convenient way to refine the mesh in the vicinity of the boundaries is to reduce the **Curvature factor** in the **Size** settings window in the mesh sequence. This results in a finer mesh only where the radius of curvature of the surface is small. You might also have to reduce the **Minimum element size** to avoid warnings in the mesh sequence.

- Features that compute the density of some quantity on a domain or boundary usually require a finer mesh, because the density term is piecewise discontinuous across elements. This includes the Accumulator (Boundary), Accumulator (Domain), and Deposited Ray Power (Boundary) features. If the mesh is too fine, rays might entirely miss some elements, and then it is necessary to increase the number of rays to avoid "holes" in the deposited power or other density field.

- Whenever possible, use parts from the Ray Optics Module Part Libraries, rather than constructing complicated shapes from geometry primitives like the sphere and cylinder. Many of these parts use high-accuracy geometry representations of the surfaces which reduce the numerical error when rays interact with them.

- When using the built-in geometry Parts for aspheric lenses or mirrors, consider enabling the built-in extra points (see the **Input Parameters** section), especially if higher-order polynomial terms are included.

- Consider changing the **Geometry shape order** in the model component settings. Using **Cubic** or **Quartic** causes the boundaries to be discretized using higher-order polynomials, which can reduce error by several orders of magnitude.

  Similarly, with physics interfaces that solve for a displacement field, such as Solid Mechanics, locate the physics interface **Discretization** section. A higher shape order such as **Cubic Lagrange** should be selected if rays are traced in the deformed geometry

- If the geometry uses parts or primitives, you can reduce discretization error by selecting **Use geometry normals for ray-boundary interactions** in the physics interface **Ray Release and Propagation** section. However, this only improves the accuracy if the geometry is undeformed; it has no effect if the geometry is subjected to thermal stress or some other type of deformation.

# Domain Properties

A fundamental step in setting up any ray optics model is identifying the material that the rays are propagating through. You can control the refractive indices of the domains in the selection for the Geometrical Optics interface. You can also control the refractive index in the empty space between the selected domains, albeit with some restrictions (see below).

## *Refractive Index*

The refractive index is a complex-valued material property. Its real part indicates the speed of light within the material; its imaginary part describes how quickly a beam will attenuate (that is, decrease in intensity) as it passes through the material.

The refractive index and other properties of domains included in the Geometrical Optics interface can be set using the Medium Properties node. It is also possible to specify the refractive index of the void surrounding a Geometrical Optics model.

### ABSOLUTE VS RELATIVE INDEX

When looking at refractive index data for a given material, it is essential to know whether the refractive index is *absolute* or *relative*:

- An absolute refractive index is defined with respect to vacuum. That is, if the absolute index of a material is 1.5, the speed of light in that material is $c/1.5$, where $c = 299{,}792{,}458$ m/s is the speed of light in a vacuum.

- A relative refractive index is defined with respect to some other material, most often air. If the relative index of a material is 1.5, then the speed of light in that material is $c/1.5$, where $c$ is the speed of light in air.

Furthermore, the speed of light in air is a function of temperature and pressure. Typically, when defining the relative refractive index, the air is at a reference temperature of 1 atm and a reference temperature of 20°C, although some glass catalogs use a different reference temperature such as 15°C.

The settings for the Medium Properties always indicate whether the specified refractive index is absolute or relative; and if the given refractive index is relative, a reference temperature and reference pressure are always shown.

During results processing, the variable `gop.nref` is always the absolute refractive index, regardless of whether the absolute or relative index was specified.

In the physics interface settings **Material Properties of Exterior and Unmeshed Domains** section, the **Optical dispersion model** is specified. This determines the **Refractive index of exterior domains, real part**. This refractive index is used in any domains outside of the selection for the Geometrical Optics interface, as well as the void domain outside the geometry. It is a spatially uniform, scalar-valued quantity. The refractive index outside the domain selection cannot depend on field variables such as temperature or pressure and cannot be a graded-index medium. For domains with temperature-dependent or spatially nonuniform refractive indices, use the Medium Properties node instead.

## Scattering and Absorption

If you specify a complex-valued refractive index and are solving for ray intensity or power (see the section Intensity, Polarization, and Power), you can make the intensity and power vary along the ray path. If the medium properties are uniform, the intensity and power usually follow exponential decay (for an absorbing medium) or growth (for a gain medium). You can switch between absorbing and gain media by changing the sign of the imaginary part of the refractive index.

An alternative way to specify the imaginary part of the refractive index is to enter a value or expression for the internal transmittance for a given thickness of the material. For example, many of the optical glasses from the Optical Material Library (see the Material Libraries section) provide tabulated values of the internal transmittance as a function of wavelength.

Usually the real and imaginary parts of the refractive index in a homogeneous medium are material properties. Sometimes, however, the absorption is due to the presence of small imperfections or particles in a medium. Some examples include dust, water droplets, or smoke in air; bubbles or sediment in water; or colloidal suspensions. In such cases, you can include the losses due to absorption and scattering by these particles using the dedicated Scattering Domain node.

# Boundary Conditions

This section describes the boundary conditions of the Geometrical Optics interface in greater detail:

- Reflection and Refraction
- Primary and Secondary Ray Releases
- Wall Conditions
- Special Boundary Conditions

## *Reflection and Refraction*

The default boundary condition is the Material Discontinuity condition on all interior and exterior boundaries. The **Material Discontinuity** causes rays to be reflected and refracted if the two adjacent domains have different refractive indices.

The direction of the refracted ray is based on Snell's law. If the ray intensity or power is solved for, then they are reinitialized according to the Fresnel equations. You can modify the application of Fresnel equations by adding one or more thin dielectric layers to the surface.

> Material Discontinuity Theory and Intensity, Wavefront Curvature, and Polarization in Theory for the Geometrical Optics Interface.

### SUPPRESSING THE RELEASE OF REFLECTED RAYS

The total number of released secondary rays in a model can sometimes grow rapidly and exhaust all of the preallocated secondary degrees of freedom. For example, a single ray reflecting back and forth between two **Material Discontinuity** boundaries can create an inordinately large number of rays, each with extremely low intensity. Remember that the total number of secondary rays that can be produced in the model is limited by the number specified in the **Maximum number of secondary rays** field.

It can be useful to constrain the release of secondary rays at boundaries so that only the most important rays are produced. If reflected rays are not of any interest, then in the **Rays to Release** section, select **Never** from the **Release reflected rays** list. If reflected rays are only relevant to the model under a certain condition, such as hitting a specific

part of the surface or having a certain direction, instead select **Based on logical expression** and then enter a user-defined **Evaluation expression** that must be satisfied.

If ray intensity is solved for, you can also specify a **Threshold intensity**. If a reflected ray would have intensity below the threshold, it is not released at all. Similarly, if ray power is solved for, you can specify a **Threshold power**.

## Primary and Secondary Ray Releases

In the Geometrical Optics interface, a ray is *released* when it begins to propagate. The physics features that control where and how rays are released are called *ray release features* or simply *release features*. These features are separated into two categories, called *primary release features* and *secondary release features*. Similarly, the rays created by each feature are either *primary rays* or *secondary rays*.

### PRIMARY RAYS

A primary release feature allows the initial position and direction of rays to be specified directly. For the release positions, either specify the grid points directly (as in the Release from Grid feature) or choose the geometric entities that produce the rays (as in the Release, Release from Boundary, Release from Edge, and Release from Point features). The initial direction can be specified directly or sampled from a distribution.

Primary rays are released directly by a release feature. They are called primary rays because their release is not contingent on the prior existence of any other ray.

### SECONDARY RAYS

Secondary rays are released when an existing ray is subjected to certain boundary conditions. This existing ray might be a primary ray, or it could be a different secondary ray that was released earlier in the simulation.

For example, the following diagram shows an incident ray being split into reflected and refracted rays at a Material Discontinuity where the refractive indices on either side differ. The Geometrical Optics interface always applies deterministic ray splitting at such boundaries, so when one ray reaches the surface, two rays emerge from it. The refracted ray is a continuation of the incident ray because it has the same index and uses the same degrees of freedom. The reflected ray is a secondary ray.

Note that total internal reflection is automatically detected. In this case the incident ray is simply reflected and no refracted ray appears. Therefore, total internal reflection does not require the release of a secondary ray.

Released (primary) ray
Reflected (secondary) ray
Material discontinuity
Refracted (primary) ray
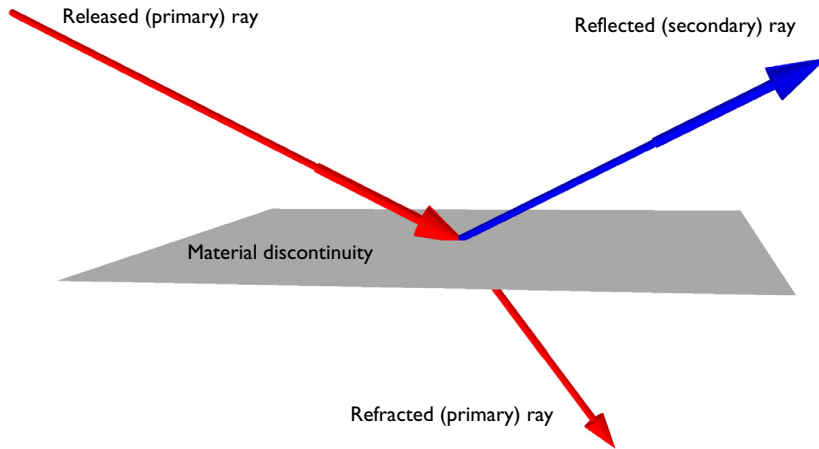
**ALLOCATION OF SECONDARY DOFS**

The number of degrees of freedom allocated to secondary rays is determined when the study begins, and if this maximum number is ever reached, then no additional secondary rays will be released. In other words, if a large number of reflected rays have been produced at material discontinuities in a model, at some point no more reflected rays will be produced. In this case, a **Warning** will appear in the solver sequence. The maximum number of secondary rays that can be produced in a model is controlled by the **Maximum number of secondary rays** field in the physics interface settings **Ray Release and Propagation** section.

Similarly, the Grating and Cross Grating boundary conditions can release both reflected and transmitted rays of many diffraction orders. One of these reflected or transmitted rays uses the degrees of freedom of the incident ray, and the rest must be taken from the preallocated secondary degrees of freedom.

| | In the *Sagnac Interferometer* example, a single ray is split up into four distinct rays due to reflection and refraction at the **Material Discontinuity**. The phase difference between two of these rays is then computed. Application Library path **Ray_Optics_Module/ Spectrometers_and_Monochromators/sagnac_interferometer** |
|---|---|

## Wall Conditions

For most boundary conditions other than refraction, the Wall feature can be used. It includes a wide variety of boundary conditions including the following:

• Specular reflection

• Diffuse reflection

• Isotropic reflection

• Combination of diffuse and specular reflection

• User-defined reflection

• Pass through

• Several varieties of absorption condition (see below)

In this context, diffuse reflection means Lambertian scattering, following the cosine law; as opposed to isotropic scattering, in which reflected light has an equal probability of being reflected in any direction to one side of the boundary.

If you choose **Mixed diffuse and specular reflection**, you can assign some probability that the ray is reflected specularly; otherwise, it is reflected diffusely.

The **Diffuse scattering** and **Mixed diffuse and specular reflection** rely on pseudorandom number generation, so they are not guaranteed to give exactly the same numerical results in different software versions or on different architectures.

### TYPES OF RAY ABSORPTION

There are several different types of absorption condition, classified by the type of information that they retain about the ray.

• The **Disappear** condition annihilates the ray completely. After the ray disappears, its position and other degrees of freedom evaluate to not-a-number (NaN).

• The **Freeze** condition retains the ray position and direction after the ray hits the boundary, although these quantities no longer change over time.

• The **Stick** condition retains the ray position, but all other degrees of freedom are set to zero.

If the model includes several different types of boundary condition and you want to know what type of condition was applied to each ray, select the **Store ray status data** check box. This will store a variable that indicates the final status of each ray: whether it has not been released yet, is still propagating, or has been absorbed.

The Wall feature also support conditional ray-wall interactions. For example, you could cause rays to **Freeze** if a logical expression is satisfied — for example, having optical path length greater than a specified threshold — and subject them to **Specular reflection** otherwise. Together with the **Mixed diffuse and specular reflection** condition, it is possible to prescribe up to 3 different types of wall interaction at a single boundary.

## Special Boundary Conditions

More specialized boundary conditions are available for some application areas.

The Grating and Cross Grating boundary conditions, together with the Diffraction Order (Grating) and Diffraction Order (Cross Grating) subnodes, respectively, are used to separate rays by diffraction at a periodic structure. The **Grating** is periodic in one direction and homogeneous in the orthogonal direction; the **Cross Grating** is periodic in two directions. Either feature can release both reflected and transmitted rays. You can specify the direction of periodicity and the size of the unit cell.

---

*Czerny-Turner Monochromator*: Application Library path
**Ray_Optics_Module/Spectrometers_and_Monochromators/czerny_turner_monochromator**

*White Pupil Échelle Spectrograph*: Application Library path
**Ray_Optics_Module/Spectrometers_and_Monochromators/white_pupil_echelle_spectrograph**

*Cross Grating Échelle Spectrograph*: Application Library path
**Ray_Optics_Module/Spectrometers_and_Monochromators/cross_grating_echelle_spectrograph**

---

The Mirror boundary condition is a simplified Wall that only causes specular reflection.

The Scattering Boundary feature can be used to scatter rays in both transmission and reflection.

The Axial Symmetry boundary condition is only available in 2D axisymmetric models. It is automatically applied at the axis of symmetry and cannot be applied anywhere else.

Optical devices like the Linear Polarizer and Linear Wave Retarder are available when ray intensity or power is computed. They do not have any effect on the ray direction but they can affect the ray polarization.

# Ray Release Features

To trace rays it is first necessary to prescribe their initial position and direction. This process is called *releasing* rays. The physics features used to enter this information are called *release features* or *ray release features*. If other quantities are being solved for along the rays, such as the intensity and polarization, then these quantities are initialized by the ray release features.

In this section:

- Grid-Based Release
- Release from Domains, Boundaries, Edges, or Points
- Specialized Release Features
- Release Features for Multiscale Modeling

## *Grid-Based Release*

Use the Release from Grid feature to specify the initial positions of rays using a grid of points. It is useful to release rays from a grid when the initial ray position is known exactly. A grid-based release may be used, for example, when rays are released from the focus of a lens or when a system is excited by a laser. This is the easiest way to release rays from known locations in the void region outside the geometry.

Alternatively, you can load the ray release positions and directions from a text file, using the Release from Data File node.

## *Release from Domains, Boundaries, Edges, or Points*

There are ray release features for every geometric entity level:

- Use the Release feature to release rays from domains in 2D or 3D.
- Use the Release from Boundary feature to release edges (2D) or surfaces (3D).
- Use the Release from Edge feature to release rays from edges in 3D.
- Use the Release from Point feature to release rays from points in 2D or 3D.

Releasing rays from a domain, surface, or edge initializes the ray position based on the underlying finite element mesh, which discretizes the geometry. A side effect is that the ray positions can change slightly when switching between geometry kernels. Ray

release can be uniform or proportional to a user-defined expression, which is specified in the **Density proportional to** text field.

## *Specialized Release Features*

The Illuminated Surface is a specialized ray release feature that produces reflected or refracted light directly at a surface. This can be used, for example, when the direction of incident radiation is known, but its propagation is not interesting until it has already been reflected once by an object.

The Solar Radiation computes the initial direction of rays as if they were solar rays being released at a specified latitude, longitude, date, and time. Instead of the latitude an longitude, you can also select from a list of built-in cities.

> The following examples involve buildings or other objects being illuminated by solar radiation in a specific direction:
>
> - *Solar Dish Receiver*: Application Library path **Ray_Optics_Module/ Solar_Radiation/solar_dish_receiver**
> - *Vdara® Caustic Surface*: Application Library path **Ray_Optics_Module/Solar_Radiation/vdara_caustic_surface**

## *Release Features for Multiscale Modeling*

The Ray Optics Module also supports multiscale electromagnetics simulation, in which the electric field is first computed in the frequency domain over a length scale of several wavelengths, then propagated over a much longer distance using a ray tracing approach. For more details, see Release from Electric Field and Release from Far-Field Radiation Pattern.

# Additional Variables Solved For

The Geometrical Optics interface always solves for the ray position **q** (SI unit: m) and wave vector **k** (SI unit: rad/m). This section lists the optional quantities that can be solved for in addition to these required variables.

In this section:

- Modeling Polychromatic Radiation
- Intensity, Polarization, and Power
- Other Dependent Variables
- Order of Initialization of Auxiliary Dependent Variables

## *Modeling Polychromatic Radiation*

By default, the rays released in a model are monochromatic with a ray frequency or free-space wavelength defined in the Ray Properties settings window. However, you can trace polychromatic rays by specifying different frequencies or vacuum wavelengths in each ray release feature.

To allow the rays to be polychromatic, in the settings window for the Geometrical Optics interface locate the **Ray Release and Propagation** section. By default, **Monochromatic** is selected from the **Wavelength distribution of released rays** list. Select **Polychromatic, specify vacuum wavelength** to release polychromatic rays by entering an expression for the vacuum wavelength or sampling it from a distribution. Alternatively, select **Polychromatic, specify frequency** to define an expression or distribution for the ray frequency. These expressions are defined in the **Vacuum Wavelength** and **Initial Ray Frequency** sections in each ray release feature.

When modeling polychromatic light, the number of degrees of freedom in the model increases by one per ray because the wavelength or frequency is stored as an auxiliary dependent variable on each ray.

|  |  |
|---|---|
| ▥ | *Czerny-Turner Monochromator*: Application Library path **Ray_Optics_Module/Spectrometers_and_Monochromators/ czerny_turner_monochromator** |

## *Intensity, Polarization, and Power*

Ray intensity is computed using a variant of the Stokes–Mueller calculus in which both the amplitude and polarization are tracked along individual rays.

### LIST OF AVAILABLE SETTINGS

To decide whether intensity is computed, select an option from the **Intensity Computation** list. The following options are available.

- **None**: Does not compute any intensity information.

- **Compute intensity**: Solves for intensity, which typically increases as rays are focused and decreases as they diverge. Also affected by reflection, refraction, and attenuating media. Only valid when the media are homogeneous.

- **Compute power**: Solves for power, which is unaffected by the convergence or divergence of rays but is still affected by reflection, refraction, and attenuating media. Can be used to compute heat source terms in attenuating domains or heat flux terms on absorbing boundaries that the rays hit.

- **Compute intensity and power**: Combines the capabilities of **Compute intensity** and **Compute power**, at the cost of a few extra degrees of freedom per ray.

- **Compute intensity in graded media**: Similar to **Compute intensity**, but is also applicable to graded-index media. The tradeoff is that this method is slower and less accurate for homogeneous media.

- **Compute intensity and power in graded media**: Similar to **Compute intensity in graded media** but can also be used to generate heat sources in attenuating domains and heat flux terms at boundaries.

### HANDLING POLARIZATION

Whenever intensity or power is solved for, the polarization of every ray is known. Rays can have any degree of polarization, ranging from 0 (unpolarized) to 1 (fully polarized) and anything in between. When rays have some degree of polarization, they can be linearly, elliptically, or circularly polarized.

When rays are reflected and refracted at boundaries, the intensity, polarization, and power are updated based on the Fresnel equations, which automatically take the polarization direction into account.

The polarization is determined based on the Stokes parameters, which are allocated as extra degrees of freedom along each ray. For more information, see The Stokes Parameters in the Theory for the Geometrical Optics Interface chapter.

In the following examples, ray polarization is manipulated in an instructive way:

- *Total Internal Reflection Thin-Film Achromatic Phase Shifter (TIRTF APS)*: Application Library path **Ray_Optics_Module/ Prisms_and_Coatings/achromatic_phase_shifter**

- *Linear Wave Retarder*: Application Library path **Ray_Optics_Module/ Tutorials/linear_wave_retarder**

### WAVEFRONT CURVATURE

When the ray intensity is solved for, it increases where rays are focused together and decreases where rays diverge. This is accomplished by treating each ray as a wavefront and storing its principal radii of curvature as extra degrees of freedom. In this way, all released rays are treated as points on planar, spherical, or ellipsoid-shaped wavefronts.

For more information on wavefront radii of curvature and their effect on intensity, see Principal Radii of Curvature in the Theory for the Geometrical Optics Interface chapter.

### COMPUTING DEPOSITED RAY POWER

The options **Compute power**, **Compute intensity and power**, and **Compute intensity and power in graded media** all allow heat sources to be defined on domains or boundaries. As rays propagate through an attenuating medium — that is, a medium where the refractive index is complex-valued — some energy is lost from the ray. The corresponding heat source on the surrounding domain can be computed using either the Deposited Ray Power (Boundary) subnode or the Ray Heat Source multiphysics node. A **Ray Heat Source** node is automatically created when you have selected The Ray Heating Interface in the Model Wizard. The heat generated as rays propagate in an attenuating medium can be used to define a heat source in the Heat Transfer in Solids interface or another physics interface that computes a temperature field.

*Thermally Induced Focal Shift in High-Power Laser Focusing Systems*: Application Library path **Ray_Optics_Module/ Structural_Thermal_Optical_Performance_Analysis/ thermally_induced_focal_shift**

The Grating feature is used to model the transmission and reflection of rays at diffraction gratings. It includes a Diffraction Order (Grating) subnode to specify which diffraction orders to release. When the ray power is solved for, the **Store total transmitted power** and **Store total reflected power** check boxes are shown in the **Grating** settings window. Selecting either of these check boxes causes an auxiliary dependent variable to be declared, storing the total power of the transmitted and reflected rays of all diffraction orders.

> *Diffraction Grating*: Application Library path **Ray_Optics_Module/ Verification_Examples/diffraction_grating**

## *Other Dependent Variables*

It is possible to define an auxiliary dependent variable for the optical path length by selecting the **Compute optical path length** check box in the **Additional Variables** section of the physics interface node's Settings window. Initially, the optical path length is set to 0 for all released rays. It is possible to reset the optical path length to 0 when the rays interact with boundaries.

The phase of a ray is necessary for some applications that require information about the instantaneous electric fields of multiple rays, such as interferometers. To define an auxiliary dependent variable for phase, select the **Compute phase** check box in the **Intensity Computation** section of the physics interface node's Settings window. This check box is only available if the ray intensity is computed.

The instantaneous phase can be used to visualize interference patterns where the rays intersect a surface. See the Results Analysis and Visualization section.

Other dependent variables can also be assigned, including:

- The number of times each ray has been reflected.
- Help variables for more accurately tracing rays in strongly absorbing media, where the real and imaginary parts of the refractive index are comparable in magnitude.
- Help variables used to apply perturbations in ray direction due to rough surfaces.
- User-defined Auxiliary Dependent Variable nodes.

*Order of Initialization of Auxiliary Dependent Variables*

When rays are released, the variables defined for each ray are initialized in a specific order. The initial values of ray variables can only depend on the values of variables that have already been defined. The order of dependent variable initialization is governed by the following rules:

- The initial ray position is always determined first.

- By default, user-defined auxiliary dependent variables (that is, those that are defined by adding an Auxiliary Dependent Variable node to the physics interface) are initialized after all other variables. They can instead be initialized immediately after the ray position vector components by selecting the **Initialize before wave vector** check box shown in the release feature **Initial Value of Auxiliary Dependent Variables** section.

- If more than one user-defined auxiliary dependent variable is present, these variables are initialized in the order in which the corresponding **Auxiliary Dependent Variable** nodes appear in the Model Builder.

- The remaining degrees of freedom are defined in the following order (each listed group is initialized simultaneously, and the variables within a group cannot reliably be initialized in terms of each other):

  - Help variable for the perturbation of initial ray direction at illuminated surfaces

  - Ray frequency or vacuum wavelength

  - The wave vector components, optical path length, and total power transmitted and reflected by gratings

  - The integral of the attenuation coefficient along ray paths and the components of the unit vector that indicates the direction corresponding to one of the principal radii of curvature

  - The principal radii of curvature, initial principal radii of curvature, intensity, Stokes parameters, and help variables for computing the curvature tensor and intensity

  - The total power transmitted by the ray

Items in each bullet point may not be initialized as functions of items in a later bullet point. For example, the initial ray direction vector can depend on the ray frequency, but the initial principal radii of curvature cannot depend on the total power transmitted by the ray.

# Study Types

The Geometrical Optics interface is compatible with three study types: **Ray Tracing**, **Time Dependent**, and **Bidirectionally Coupled Ray Tracing**. In this section some of the more relevant study settings are explored in greater detail.

In this section:

## *Ray Tracing Study Step*

The **Ray Tracing** and **Time Dependent** study steps are very similar, and either one could be used for the vast majority of geometrical optics models. The **Ray Tracing** study step has some additional features that make it more convenient to use, such as more reasonable default values and built-in stop conditions.

### A NOTE ON GEOMETRIC NONLINEARITY

If a physics interface solves for the displacement field, such as the Solid Mechanics interface, then the **Include geometric nonlinearity** check box appears in the **Study Settings** section. It is very important to select this check box when tracing rays in a system that is deformed due to external forces or thermal stress. If the check box is cleared, then rays are instead traced in the undeformed geometry.

### TIME STEPS AND OPTICAL PATH LENGTH INTERVALS

By default, the **Ray Tracing** study step computes ray trajectories from $t = 0$ to $t = 1$ ns with a time step size of $0.01$ ns. However, it is often useful to think of ray tracing in terms of the maximum distance of ray propagation instead of the maximum time. To express the duration of the study in terms of a maximum optical path length, change the **Time step specification** setting from the default, **Specify time steps**, to **Specify maximum path length**. Then select a **Length unit** (default: m), enter a set of **Lengths** (default: `range(0,0.01,1)`), and enter a **Characteristic group velocity** (default: `c_const`, a built-in constant for the speed of light in a vacuum). With the default solver settings, the time-dependent solver must take at least one time step whenever the optical path length of a ray moving at the **Characteristic group velocity** would have reached one of the values in the list of **Lengths**.

**BUILT-IN STOP CONDITIONS**

The **Ray Tracing** study step includes options to create a **Stop Condition** node in the default solver sequence. The **Stop Condition** node can terminate the study before the full range of specified times or optical path lengths has been simulated, if a condition is met before then.

To use one of the built-in stop conditions, select one of the following options from the **Stop condition** list in the **Study Settings**:

- **None**: The study ends at the specified maximum time or maximum optical path length.
- **No active rays remaining**: The study terminates if all rays have been stopped or absorbed. A ray can be absorbed by a boundary, or it can be removed by the Ray Termination domain feature.
- **Active rays have intensity below threshold**: This option is only available when ray intensity is computed. The study terminates if every ray in the model is either stopped, absorbed, or has sufficiently low intensity.
- **Active rays exceed maximum number of reflections**: This option is only usable when the **Count reflections** check box is selected in the physics interface settings **Additional Variables** section. The study terminates if every ray in the model is either stopped, absorbed, or has been reflected the specified number of times.

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| | |
|---|---|
| 🔍 | Stop Condition in the *COMSOL Multiphysics Reference Manual*. |

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**COUPLED PHYSICS INTERFACES**

If other physics interfaces are also solved for in the **Ray Tracing** study step, it is assumed that these other fields vary over the same time scale as the ray propagation. This is seldom true. If, instead, the coupled physics do not change over the time scale for ray propagation, consider a study with two steps: **Stationary** for all other fields and **Ray Tracing** just for the rays.

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| | |
|---|---|
| 🔍 | In the *COMSOL Multiphysics Reference Manual*:<br>- Ray Tracing<br>- Studies and Solvers |

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## Bidirectionally Coupled Ray Tracing Study Step

The **Bidirectionally Coupled Ray Tracing** study step is a dedicated study step for ray heating and similar applications.

It should only be used if all of the following criteria are met:

1 Rays are being traced.

2 Some other field, such as temperature or structural displacement, is solved for in a domain where the rays are being traced.

3 All fields, apart from the ray paths themselves, are stationary.

4 The ray paths are affected by the field being solved for. This could include rays interacting with a deformed geometry, or a refractive index that depends on the values of field variables like strain or temperature.

5 The rays generate enough heat to significantly affect one of the fields being solved for in the domain, usually temperature.

If condition 4 is not satisfied, instead use a **Stationary** study step for the fields, followed by a **Ray Tracing** study step for the rays.

In addition to the settings that are available for the **Ray Tracing** study step, it is possible to specify a **Number of iterations**. The default value is 5. If the **Bidirectionally Coupled Ray Tracing** study step is used with The Ray Heating Interface, the following iterative solver loop is automatically set up to compute the ray trajectories and temperature:

1 Solve for the temperature field, assuming that the rays do not generate any heat source.

2 Using the temperature computed during the previous step, compute the ray paths and any heat sources that occur due to ray attenuation in an absorbing medium.

3 Using the heat source computed in the previous step, compute the temperature field.

4 Alternate between Steps 2 and 3 for the specified **Number of iterations**, or specify a **Global variable** whose convergence will be used to terminate the loop.

The result of the iterative solver loop is that the heat source generated by the attenuation of rays is taken into account when computing the temperature. By including a thermo-optic dispersion model, such as the **Temperature-dependent Sellmeier** model, the temperature in turn affects the ray paths. Thus, a bidirectional coupling is established between the two physics interfaces.

Like any COMSOL Multiphysics simulation, it is possible to extend this bidirectional coupling to include other physical effects. For example, to include structural deformation due to thermal stress, add the Solid Mechanics physics interface and the **Thermal Expansion** Multiphysics coupling.

| | |
|---|---|
| ▥ | *Thermally Induced Focal Shift in High-Power Laser Focusing Systems*: Application Library path **Ray_Optics_Module/ Structural_Thermal_Optical_Performance_Analysis/ thermally_induced_focal_shift** |

| | |
|---|---|
| ⌕ | In the *COMSOL Multiphysics Reference Manual*: <br> • Bidirectionally Coupled Ray Tracing <br> • Studies and Solvers |

# Results Analysis and Visualization

The results of a ray tracing simulation can be interpreted and visualized using a variety of built-in features. In the following, some dedicated features are discussed in detail.

In this section:

- Ray Trajectories Plot
- Ray Plot
- Interference Pattern Plot
- Spot Diagram Plot
- Optical Aberration Plot and Aberration Evaluation
- Plotting Refractive Index and Abbe Number

## Ray Trajectories Plot

The default **Ray Trajectories** plot shows each ray as a line, ribbon, or tube. The final ray position can be rendered as a point or vector. It is also possible to modify the **Ray Trajectories** plot by adding **Color Expression**, **Deformation**, **Material Appearance**, **Filter**, **Translation**, or **Transparency** attributes (subnodes).

As an example, when the ray intensity is computed, you can also plot polarization ellipses along the ray paths, using the built-in variables (gop.pax, gop.pay, gop.paz) for the semi-major axis and (gop.pbx, gop.pby, gop.pbz) for the semi-minor axis.
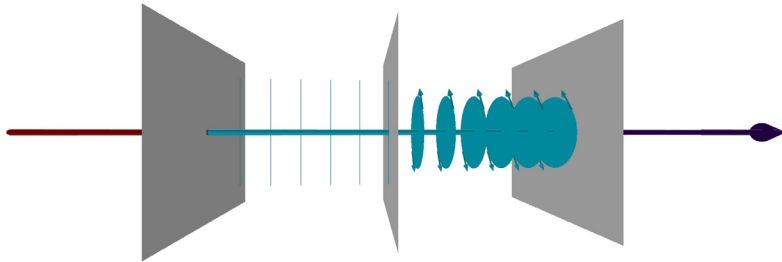


*Figure 2-3: Polarization ellipses as a ray crosses a linear polarizer, linear wave retarder, and a second linear polarizer.*

| | *Linear Wave Retarder*: Application Library path **Ray_Optics_Module/ Tutorials/linear_wave_retarder** |
|---|---|

*Ray Plot*

The **Ray** plot can be added to 1D plot groups. There are two primary ways to use this plot:

**1** Plot an expression versus time for all rays, or as a data series operation such as a sum or average over all rays.

**2** Plot two expressions against each other, creating a separate curve for each ray, at a specified time.

The following plot is an example of usage case 2. Polychromatic light is transmitted through a multilayer film, and then the intensity at the final time step is plotted against vacuum wavelength for all rays.
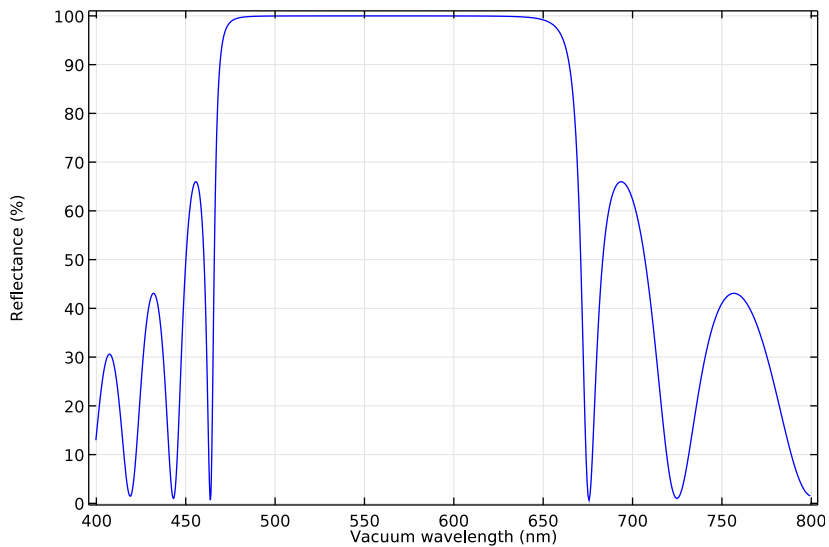


*Figure 2-4: Reflectance of a distributed Bragg reflector with 21 dielectric layers is plotted as a function of free-space wavelength.*

| | |
|---|---|
| ▥ | *Distributed Bragg Reflector*: Application Library path **Ray_Optics_Module/Prisms_and_Coatings/distributed_bragg_reflector** |

## Interference Pattern Plot

The pattern of fringes resulting from the interference of two or more rays can be plotted using the dedicated **Interference Pattern** plot. The Interference Pattern plot is available in 2D plot groups and requires a **Cut Plane** dataset pointing to a **Ray** dataset. The interference pattern is then plotted using the locations and properties of rays as they intersect the cut plane.
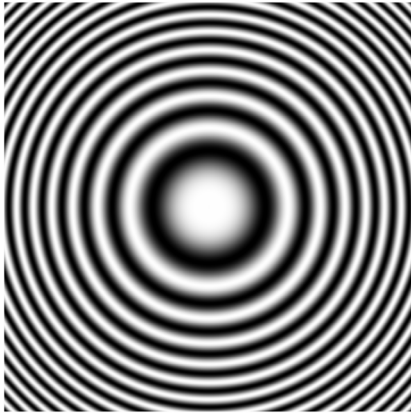


*Figure 2-5: Interference pattern resulting from two point sources at slightly different distances from a surface.*

The **Interference Pattern** can only be plotted if the ray intensity and phase are solved for; in the physics interface settings, select an appropriate intensity computation method from the **Intensity computation** list, then select the **Compute phase** check box.

For the resulting interference pattern to be physically meaningful, it must be plotted over a region with a length scale that is much smaller than the principal radii of curvature of the incident wavefronts. This is equivalent to the assumption that the wavefront associated with each ray subtends a very small solid angle, and is necessary due to the approximation used to compute the incident intensity.

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     Interference Pattern Theory

*Spot Diagram Plot*

After tracing rays in 3D, you can plot the intersection points of rays with a surface using the dedicated **Spot Diagram** plot. This plot can only be added to a **2D Plot Group**. The **Spot Diagram** includes many options for filtering and sorting the intersection points. It can also automatically locate a plane of best focus, and add text annotations.

The **Spot Diagram** can either use a **Ray** dataset, in which case it plots all applicable rays at the same time, or an **Intersection Point 3D** dataset, where the intersection points with a surface are plotted.
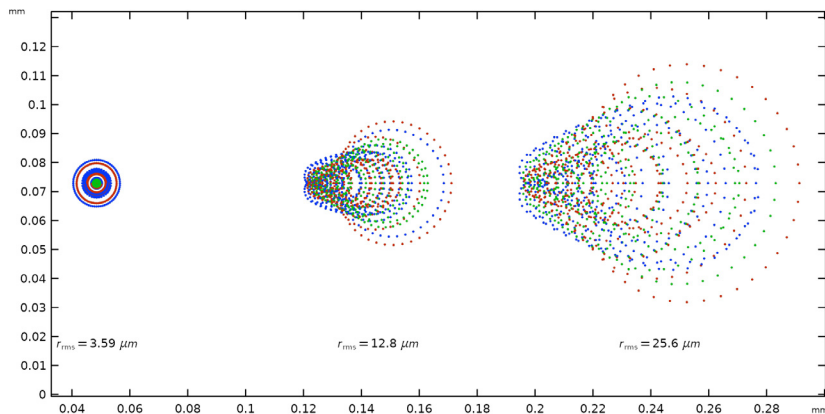


*Figure 2-6: Spot diagrams for a Schmidt–Cassegrain telescope at three different field angles. The color expression indicates the wavelength.*

### FILTERING RAYS

Use the **Filters** section to show or hide certain rays. This section contains check boxes for different filter criteria. You can select several of these check boxes at once, and rays will only be shown if they satisfy all of the selected criteria.



*Figure 2-7: Filter options for the Spot Diagram plot.*

For example, you can select **Filter by wavelength** to hide rays of all wavelengths except a selected value; then select **Filter by release feature index** to only show rays that are released by a specific feature (for example, **Release from Grid 1**). In many examples of cameras and telescopes in the Application Libraries, each release feature corresponds to a distinct field angle for light entering the optical system.

The **Filter by number of reflections** check box should only be used if you previously selected **Count reflections** in the physics interface **Additional Variables** section.

### CREATING AND ORGANIZING AN ARRAY OF SPOTS

Use the **Layout** section to organize rays into different spots based on release feature or wavelength. If the model has multiple wavelengths or release features, this could result in an array of different spots being plotted at the same time. This section also has settings for the positioning of these different spots relative to each other in the Graphics window. For example, you can adjust the **Horizontal padding factor** to increase the horizontal spacing between the spots.
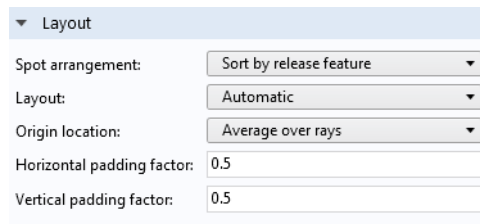


*Figure 2-8: Layout options for the Spot Diagram plot.*
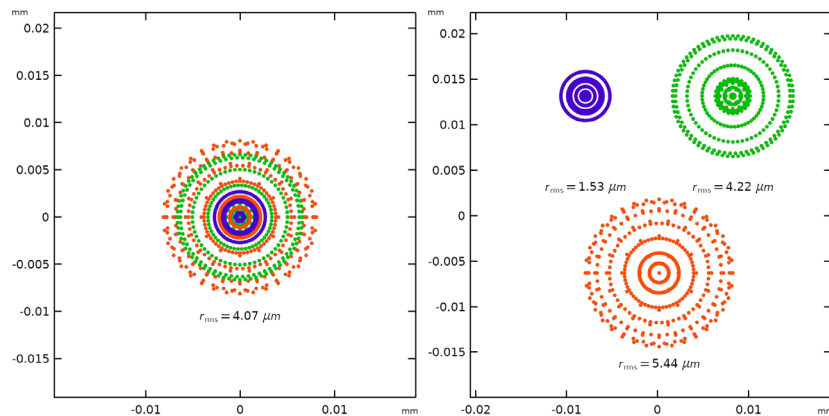


*Figure 2-9: Spot diagrams of a Petzval lens system, with three different wavelengths in the same spot (left) or sorted into separate spots for each wavelength (right).*

The **Focal Plane Orientation** section can be used to automatically locate a plane of best focus for the optical system. When you click **Create Focal Plane Dataset**, an **Intersection Point 3D** dataset will be created at a local minimum of the root mean square (rms) spot size. If the rays stop at a surface in the model and the plane of best focus is behind this surface, the automatic focal plane calculation might fail. Consider deleting the absorbing boundary, or replacing it with a **Wall** with the **Pass through** condition.
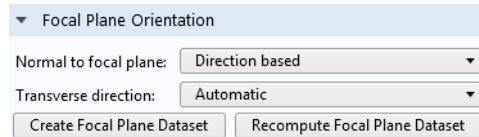


*Figure 2-10: Focal Plane Orientation options for the Spot Diagram plot.*

### ADDING TEXT ANNOTATIONS TO A SPOT DIAGRAM

The **Annotations** section can add text above or below the spots in the Graphics window. These annotations can show the position, rms spot size, and wavelength (or wavelength range) of each spot. There is also an option to draw a circle in the plot, which could be used to draw the Airy disk for scale.
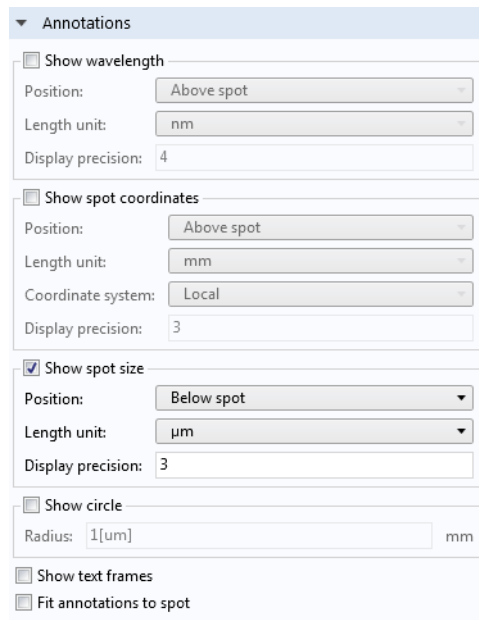


*Figure 2-11: Annotations settings for the Spot Diagram plot.*

## Optical Aberration Plot and Aberration Evaluation

The **Optical Aberration** plot can be added in a **2D Plot Group** whereas the **Aberration Evaluation** node is available under **Derived Values**. Both of these postprocessing features serve a similar purpose: to quantify the monochromatic aberrations of an imaging system and express them in terms of Zernike polynomial coefficients. In order to use the **Optical Aberration** plot, the following prerequisites must be met:

- The model component must be 3D.

- An instance of the Geometrical Optics interface must be present and solved for.

- The **Compute optical path length** check box must be selected in the Geometrical Optics **Settings** window before solving.

- An **Intersection Point 3D** dataset must be created. This dataset must point to a **Ray** dataset. Optionally, this dataset can be automatically generated (see below). In the Settings window for the **Intersection Point 3D** dataset, **Hemisphere** must be selected from the **Surface type** list. The **Center** is the location of the focus and the **Axis direction** points from the focus toward the center of the exit pupil.

Using the hemisphere defined in the **Intersection Point 3D** dataset, a Gaussian reference sphere is defined. The optical path difference among intersection points with this sphere is then expressed as a sum of Zernike polynomials.

### AUTOMATIC DATASET GENERATION

Alternatively, using the **Optical Aberration** plot, you can use the **Create Reference Hemisphere Dataset** button in the **Focal Plane Orientation** section to automatically generate a reference hemisphere at the location of the rms focus. However, note that the defocus term $Z(2,0)$ might be larger for the rms focus than it would for some other definitions of the image plane, such as the marginal focus.

The monochromatic aberrations in a double Gauss lens system are shown in Figure 2-12. The circle on the left shows the sum of all Zernike coefficients. The circle on the right ignores the defocus term $Z(2,0)$ and the piston term $Z(0,0)$. Usually, lower-order Zernike terms can be reduced by correcting misalignments in the optical system or adjusting the nominal focus. Higher-order terms are consequences of the type of lens or mirror used in an optical system; for example, a single spherical lens will always demonstrate some spherical aberration, for any position of the nominal focus.

The **Optical Aberration** plot always shows the optical path differences on a unit circle. The color expression is the wavefront error in microns. In the circle on the right in Figure 2-12, the largest contribution is from the spherical aberration term $Z(4,0)$.
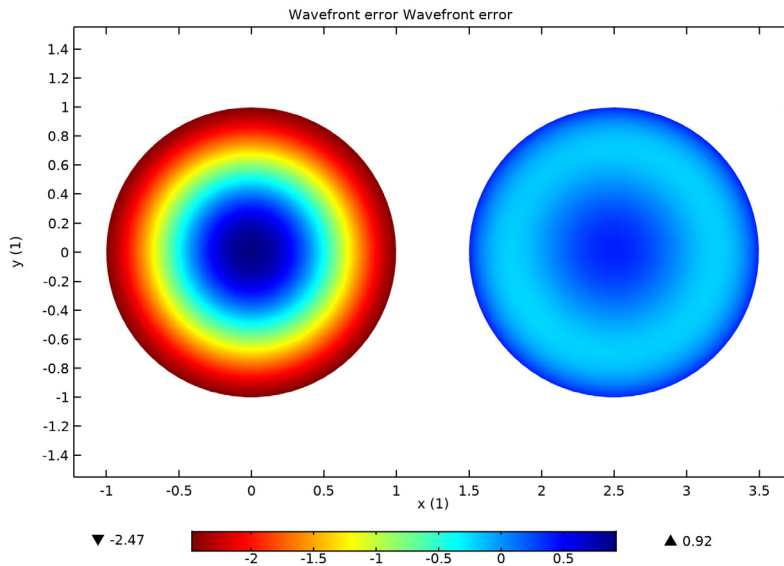
*Figure 2-12: Monochromatic aberrations in a double Gauss lens system.*

| | |
|---|---|
| 🔍 | For a list of Zernike polynomials and their derivation, see Monochromatic Aberrations and the Zernike Polynomials in Theory for the Geometrical Optics Interface. |

| | |
|---|---|
| ▥ | *Double Gauss Lens*: Application Library path **Ray_Optics_Module/ Lenses_Cameras_and_Telescopes/double_gauss_lens** |

## *Plotting Refractive Index and Abbe Number*

When trying to plot the refractive index and dispersion of materials in a Geometrical Optics model, users frequently encounter two challenges:

• There is a specific syntax that controls which variables are defined in domains, and which variables are defined only on the rays that pass through the domains.

• Real-world media are dispersive (their refractive indices depend on wavelength), so there is not just a single numeric value of the refractive index at each location.

For an instance of the Geometrical Optics interface with the default name `gop`, the variable for refractive index defined on rays is `gop.nref`, while the variable for refractive index in the domain is called `gop.nref_local`. As the rays propagate through domains in the geometry, the value of `gop.nref` is determined by evaluating `gop.nref_local` at a geometry point corresponding to each ray's current location.

Similarly, when a ray is refracted at the boundary between two different media, the implementation of Snell's law requires the variable `gop.nref_local` to be evaluated in the media on the side of the incident ray and the refracted ray, at the point where the incident ray intersects the boundary.

During postprocessing, a ray variable such as `gop.nref` can only be evaluated on rays, not at arbitrary points in the geometry where a ray might not be present. For example, trying to use `gop.nref` in a **Slice** plot will usually result in an error message such as:

```
Cannot evaluate expression.

Undefined variable.
 - Variable: comp1.gop.nref
 - Geometry: geom1
 - Domains: 1
Failed to evaluate expression.
 - Expression: comp1.gop.nref
 - Plot: Slice 1
```

A better choice for the **Slice** plot would be the variable `gop.nref_local`, which is a domain variable and therefore exists at every point in the domain, regardless of whether a ray is present there or not.

However, a **Slice** plot of `gop.nref_local` will not always work. The plot will appear correctly if the refractive index is entered as a constant value in each domain; that is, if dispersion is neglected. If the model uses optical dispersion relations that define the refractive index as a function of the wavelength of the rays, you may get an error message such as:

```
Illegal operator context.

Failed to evaluate expression.
 - Expression: noenv(comp1.gop.lambda0)
Failed to evaluate variable.
 - Variable: comp1.gop.mp1.lambda0
 - Defined as: noenv(comp1.gop.lambda0)
```

A more reliable means of plotting the refractive index of dispersive media is presented in the next section.

**EVALUATION OF REFRACTIVE INDEX OF DISPERSIVE MEDIA**

All real materials exhibit some degree of optical dispersion, or wavelength dependence of the refractive index. You can enter a value or expression for the refractive index directly, define a function (such as an **Analytic**, **Interpolation**, or **Piecewise** function), or use one of the built-in dispersion relations such as the Sellmeier dispersion formula.

In addition, the Geometrical Optics interface may be configured to trace either monochromatic or polychromatic light, by selecting the desired option from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** list.

Most of the optical glass material data in the Optical Material Libraries use a dispersion formula to define the refractive index. (See Material Libraries for a more comprehensive list of the available materials.) For example, if the Sellmeier dispersion formula is used, then the variable `gop.nref_local` is defined as

```
gop.nref_local = sqrt(1
+gop.ODsma1*gop.lambda0norm^2/(gop.lambda0norm^2-gop.ODsma4)
+gop.ODsma2*gop.lambda0norm^2/(gop.lambda0norm^2-gop.ODsma5)
+gop.ODsma3*gop.lambda0norm^2/(gop.lambda0norm^2-gop.ODsma6)
)
```

where the variables `gop.ODsma<1,2,3,4,5,6>` are the Sellmeier dispersion coefficients.

---

📄  For many commercial optical glasses, the dispersion formula defines the refractive index relative to air at a specified temperature and pressure, and then this so-called relative refractive index is automatically converted to an absolute refractive index with respect to vacuum. Here the conversion between relative and absolute index has been omitted for brevity.

---

The variable `gop.lambda0norm` is the vacuum wavelength of the ray expressed in micrometers,

```
gop.lambda0norm = gop.mp1.lambda0/1[um]
```

and this scoped variable `gop.mp1.lambda0` is defined as

```
gop.mp1.lambda0 = noenv(gop.lambda0)
```

The special operator `noenv()` allows a two-way exchange of information between the ray and the domain it is in, for the purpose of evaluating variables. It allows a ray variable (such as the wavelength) to be used in the definition of a domain variable, which in turn can be evaluated at the ray's location. However, this construction only

works if the domain variable is evaluated at the location of a ray, not at any arbitrary location in the geometry, which is why a **Slice** plot of `gop.nref_local` fails for dispersive media.

The Medium Properties node automatically defines domain variables for the refractive index at several spectral lines:

- `gop.nrefd` is the refractive index at the helium d-line, a yellow spectral line of helium with a wavelength of approximately 587.56 μm.
- `gop.nrefF` is the refractive index at the hydrogen F-line, a blue spectral line of hydrogen with a wavelength of approximately 486.13 μm.
- `gop.nrefC` is the refractive index at the hydrogen C-line, a red spectral line of hydrogen with a wavelength of approximately 656.28 μm.

The Abbe number `gop.Vd` is also available as a built-in postprocessing variable. Its definition is

```
gop.Vd=(gop.nrefd-1)/(gop.nrefF-gop.nrefC)
```

For displaying the refractive index in **Slice** or **Volume** plots, these variables for refractive index at specific wavelength values can be used more reliably than `gop.nref_local`.

Alternatively, you can evaluate the refractive index of a dispersive medium at any other wavelength value using the `subst()` operator, which can replace the ray wavelength in the dispersion formula with a fixed value. For example, another way to plot the d-line refractive index (rather than the built-in variable `gop.nrefd`) is using the expression

```
subst(gop.nref_local,gop.mp1.lambda0,587.56[nm])
```

where the third argument to the `subst()` operator could be replaced with any other numeric value.

### SUMMARY OF AVAILABLE VARIABLES

The built-in postprocessing variables `gop.nrefd`, `gop.nrefF`, and `gop.nrefC` can be used to plot the refractive indices of all materials at fixed wavelengths of 587.56 μm, 486.13 μm, and 656.28 μm, respectively. The built-in variable `gop.Vd` is the Abbe number in terms of the refractive indices at these three wavelengths. You can also plot the refractive indices of domains at any other fixed value of the wavelength using an expression of the form

```
subst(gop.nref_local,gop.mp1.lambda0,<wavelength>)
```

where `<wavelength>` should be replaced with a numeric value.

In the *COMSOL Multiphysics Reference Manual*:

- Spot Diagram
- Interference Pattern
- Optical Aberration
- Aberration Evaluation
- Ray (Plot)
- Ray Trajectories
- Filter for Ray and Ray Trajectories
- Phase Portrait
- Poincaré Map
- Ray (Dataset) and Datasets
- Ray Bin
- Intersection Point 2D and Intersection Point 3D
- Ray Evaluation and Derived Values, Evaluation Groups, and Tables
- Plot Groups and Plots

# Variables and Nonlocal Couplings

This section lists some built-in nonlocal couplings and variables for the Geometrical Optics interface.

In this section:

- Ray Statistics
- Global Variables
- Variables for Average Ray Position
- Using Ray Detectors
- Nonlocal Couplings

## *Ray Statistics*

The Geometrical Optics interface defines a number of special variables, some of which can only be used during results processing. These variables can be found in the **Ray statistics** section in the **Add/Replace Expression** menus.

In the variable names below, `gop` is the physics interface tag. If multiple instances of the Geometrical Optics interface are different, this tag may differ.

The following variables are defined for each ray:

- Ray index `gop.pidx`. Each ray is assigned a unique index starting from 1 up to the total number of rays. This expression can be used as an input argument to a function. For example, `randomnormal(gop.pidx)` would sample pseudorandom numbers from a normal distribution with unit variance. The random numbers would be distinct for each ray.

- Ray release feature `gop.prf`. If there are multiple release features in a model, it is useful to visualize which rays correspond to each release feature. Rays from each release feature are assigned a unique integer, starting at 1. This variable can also be used to filter ray trajectories in postprocessing so that only the rays released by a specific feature are shown.

- Ray release time `gop.prt`. Usually, all primary rays are released at $t = 0$. To allow other release times to be specified, select the **Allow multiple release times** check box in the physics interface **Advanced Settings** section.

If the **Store ray status data** check box is selected in the physics interface **Additional Variables** section, then the following additional variables are created:

- The release time of a given ray (variable name `gop.rti`). Unlike `gop.prt`, this works for secondary rays and thus allows for extraction of the time at which a secondary ray was released. This includes reflected rays at material discontinuities and higher diffraction orders at gratings.

- Stop time `gop.st`, when a ray gets absorbed at a boundary or annihilated by the Ray Termination feature.

- Final status `gop.fs`. This indicates the status of a ray at a given point in time. When used during postprocessing, the value always indicates the status of the ray at the last time step. The value is an integer that has one of the following values:

  - 0 for unreleased rays.

  - 1 for rays that are still propagating.

  - 2 for frozen rays.

  - 3 for stuck rays.

  - 4 for rays that have disappeared.

*Global Variables*

The following quantities can be evaluated globally, using the **Global** plot or **Global Evaluation** feature. They could be used in a **Ray Evaluation**, but they would just give the same value for every ray.

- Total number of rays, `gop.Nt`. This total includes both primary and secondary rays, and includes rays that have disappeared or have not been released.

- Total number of rays in selection, `gop.Nsel`. If a selection has been applied to the **Ray** dataset, the number of rays in that selection can be evaluated.

- Transmission probability, `gop.alpha` is the ratio of the number of rays in a selection to the total number of rays.

For each ray release feature, the total number of rays released by feature is also defined. This variable has physics feature scope, so, for example, a Release from Grid node with tag `relg1` would define a variable called `gop.relg1.Ntf`.

This global variable is uniquely defined for each release feature and gives the total number of rays that are released by that feature. This includes rays that have disappeared or have otherwise stopped propagating due to interaction with the surrounding boundaries. It does not include any secondary rays.

## Variables for Average Ray Position

Some other variables for average ray position, both absolute and relative, are also defined. These variables exist with both physics scope and physics feature scope; for example, the variable `gop.rrms` is the RMS spot size for all rays in the model, but `gop.relg1.rrms` is the RMS spot size only for rays produced by **Release from Grid 1**.

- Components of the average ray position `gop.qavex`, `gop.qavey`, and `gop.qavez`, which are simple arithmetic means over the respective ray coordinates.

- Relative ray position `gop.deltaqx`, `gop.deltaqy`, and `gop.deltaqz`. These are the ray positions relative to the average ray position. for example, the relative $x$-component `gop.deltaqx` is `qx-gop.qavex`.

- RMS spot size `gop.rrms`.

- Maximum relative radial position `gop.rmaxall`.

## Using Ray Detectors

A Ray Detector is a domain or boundary feature that provides information about rays arriving on a set of selected domains or surfaces from a release feature. The feature provides convenient expressions that can be used in the **Filter** attribute of the **Ray Trajectories** plot, which allows only the rays which reach the ray detector selection to be shown. The following variables are defined by the **Ray Detector** feature, assuming a physics interface with tag `gop` and a detector with tag `rd1`:

- `gop.rd1.Ntf` is number of transmitted rays from the release feature to the ray detector at the end of the simulation.

- `gop.rd1.alpha` is the transmission probability from the release feature to the ray detector.

- `gop.rd1.rL` is a logical expression for ray inclusion. This can be set in the **Filter** node of the **Ray Trajectories** plot in order to visualize the rays which connect the release feature to the detector.

The **Ray Detector** feature defines new variables but does not otherwise affect the solution. Therefore, you can add a **Ray Detector** to a completed model and evaluate the variables it defines without recomputing the solution. To do so, right-click the **Study** node and select **Update Solution**. The new variables described above will be immediately available for results processing.

## Nonlocal Couplings

The purpose of a model is often to compute the sum, average, maximum value, or minimum value of a quantity over a group of rays, such as the average intensity or the maximum path length. An instance of the Geometrical Optics interface with physics interface tag gop creates the following nonlocal couplings:

> 📑 The built-in nonlocal coupling names have recently changed, but the couplings with the old names are still available. In their descriptions, the couplings with the old names are marked as "deprecated". Both the old and new names are listed in Table 2-1.

- gop.sum(expr) evaluates the sum of the expression expr over the rays. The sum includes all rays that are active, frozen, or stuck to boundaries. It excludes rays that have not yet been released and those that have disappeared.

- gop.sum_all(expr) evaluates the sum of the expression expr over all rays, including rays those that are not yet released or have disappeared. Since the coordinates of unreleased and disappeared rays are not-a-number (NaN), the sum may return NaN if the model includes unreleased or disappeared rays. An expression such as gop.sum_all(isnan(qx)) can be used to compute the total number of unreleased and disappeared rays.

- gop.ave(expr) evaluates the average of the expression expr over the active, frozen, and stuck rays. Unreleased and disappeared rays contribute to neither the numerator nor the denominator of the arithmetic mean.

- gop.ave_all(expr) evaluates the average of the expression expr over all rays. It is likely to return NaN if the model includes unreleased or disappeared rays.

- gop.max(expr) evaluates the maximum value of the expression expr over all active, frozen, and stuck rays.

- gop.max_all(expr) evaluates the maximum value of the expression expr over all rays.

  The treatment of NaN values in nonlocal maximum couplings can be platform-dependent, so use caution when evaluating the maximum over all rays including disappeared and unreleased rays.

- gop.min(expr) evaluates the minimum value of the expression expr over the active, frozen, and stuck rays.

- `gop.min_all(expr)` evaluates the minimum value of the expression `expr` over all rays.

  The treatment of `NaN` values in nonlocal minimum couplings can be platform-dependent, so use caution when evaluating the minimum over all rays including disappeared and unreleased rays.

- `gop.max(expr, evalExpr)` evaluates the expression `evalExpr` for the ray that has the maximum value of the expression `expr` out of all active, frozen, and stuck rays. For example, the expression `gop.max(gop.I, qx)` would evaluate the $x$-coordinate `qx` of the ray with the greatest intensity `gop.I`.

- `gop.max_all(expr, evalExpr)` evaluates the expression `evalExpr` for the ray that has the maximum value of the expression `expr` for all rays, including disappeared and unreleased rays.

- `gop.min(expr, evalExpr)` evaluates the expression `evalExpr` for the ray that has the minimum value of the expression `expr` out of all active, frozen, and stuck rays. For example, the expression `gop.min(gop.I, qx)` would evaluate the $x$-coordinate `qx` of the ray with the minimum intensity `gop.I`.

- `gop.min_all(expr, evalExpr)` evaluates the expression `evalExpr` for the ray that has the minimum value of the expression `expr` for all rays, including disappeared and unreleased rays.

The built-in nonlocal couplings are summarized in Table 2-1.

TABLE 2-1: BUILT-IN NONLOCAL COUPLINGS FOR THE GEOMETRICAL OPTICS INTERFACE

| NAME | DEPRECATED NAME | DESCRIPTION |
|---|---|---|
| `gop.sum(a)` | `gop.gopop1(a)` | Sum over rays |
| `gop.sum_all(a)` | `gop.gopop_all1(a)` | Sum over all rays |
| `gop.ave(a)` | `gop.gopaveop1(a)` | Average over rays |
| `gop.ave_all(a)` | `gop.gopaveop_all1(a)` | Average over all rays |
| `gop.max(a)` | `gop.gopmaxop1(a)` | Maximum over rays |
| `gop.max_all(a)` | `gop.gopmaxop_all1(a)` | Maximum over all rays |
| `gop.min(a)` | `gop.gopminop1(a)` | Minimum over rays |
| `gop.min_all(a)` | `gop.gopminop_all1(a)` | Minimum over all rays |
| `gop.max(a,b)` | `gop.gopmaxop1(a,b)` | At maximum over rays |
| `gop.max_all(a,b)` | `gop.gopmaxop_all1(a,b)` | At maximum over all rays |
| `gop.min(a,b)` | `gop.gopminop1(a,b)` | At minimum over rays |
| `gop.min_all(a,b)` | `gop.gopminop_all1(a,b)` | At minimum over all rays |

# Material Libraries

The Ray Optics Module features a material library with material properties for optical glasses, metals, polymers, gases, and other compounds to assist in ray optics simulation.

The Optical material library contains material property data from the following companies' products:

### CDGM GLASS CO., LTD

H-FK61, H-FK61B, H-FK71, H-FK95N, H-QK1, H-QK3L, H-K1, H-K2, H-K3, H-K5, H-K6, H-K7, H-K8, H-K9L, H-K9LGT, H-K9L*, H-K9LA, H-K10, H-K11, H-K12, H-K50, H-K51, H-ZPK1A, H-ZPK2A, H-ZPK3, H-ZPK5, H-ZPK7, H-BaK1, H-BaK2, H-BaK3, H-BaK4, H-BaK5, H-BaK6, H-BaK7, H-BaK7GT, H-BaK7A, H-BaK8, H-ZK1, H-ZK2, H-ZK3, H-ZK3A, H-ZK4, H-ZK5, H-ZK6, H-ZK7, H-ZK7A, H-ZK8, H-ZK9B, H-ZK9A, H-ZK10, H-ZK10L, H-ZK11, H-ZK14, H-ZK20, H-ZK21, H-ZK50, H-ZK50GT, H-LaK1, H-LaK2A, H-LaK3, H-LaK4L, H-LaK5A, H-LaK6A, H-LaK7A, H-LaK8B, H-LaK8A, H-LaK10, H-LaK11, H-LaK12, H-LaK50A, H-LaK51A, H-LaK52, H-LaK53B, H-LaK53A, H-LaK54, H-LaK59A, H-LaK61, H-LaK67, H-KF6, H-QF1, H-QF3, H-QF6A, H-QF8, H-QF14, H-QF50, H-QF50A, H-QF56, H-F1, H-F2, H-F3, H-F4, H-F5, H-F13, H-F51, H-BaF2, H-BaF3, H-BaF4, H-BaF5, H-BaF6, H-BaF7, H-BaF8, H-ZBaF1, H-ZBaF3, H-ZBaF4, H-ZBaF5, H-ZBaF16, H-ZBaF20, H-ZBaF21, H-ZBaF50, H-ZBaF52, H-ZF1A, H-ZF1, H-ZF2, H-ZF3, H-ZF4A, H-ZF4AGT, H-ZF5, H-ZF6, H-ZF7LA, H-ZF7LAGT, H-ZF10, H-ZF11, H-ZF12, H-ZF13, H-ZF13GT, H-ZF39, H-ZF50, H-ZF52, H-ZF52GT, H-ZF52TT, H-ZF62, H-ZF62GT, H-ZF71, H-ZF71GT, H-ZF72A, H-ZF72AGT, H-ZF73, H-ZF73GT, H-ZF88, H-ZF88GT, H-LaF1, H-LaF2, H-LaF3B, H-LaF4, H-LaF4GT, H-LaFL5, H-LaF6LA, H-LaF7, H-LaF10LA, H-LaF50B, H-LaF51, H-LaF52, H-LaF53, H-LaF54, H-LaF55, H-LaF62, H-ZLaF1, H-ZLaF2A, H-ZLaF3, H-ZLaF4LA, H-ZLaF4LB, H-ZLaF50E, H-ZLaF50D, H-ZLaF51, H-ZLaF52A, H-ZLaF52, H-ZLaF53B, H-ZLaF53BGT, H-ZLaF55D, H-ZLaF56B, H-ZLaF66, H-ZLaF66GT, H-ZLaF68C, H-ZLaF68N, H-ZLaF69, H-ZLaF69A, H-ZLaF71, H-ZLaF71AGT, H-ZLaF73, H-ZLaF75A, H-ZLaF75B, H-ZLaF76, H-ZLaF76A, H-ZLaF78B, H-ZLaF89L, H-ZLaF90, H-ZLaF92, H-TF3L, H-TF5, D-FK61, D-FK61A, D-FK95, D-QK3L, D-K9, D-K9GT, D-K59, D-PK3, D-ZPK1A, D-ZPK3, D-ZPK5, D-ZPK7, D-ZK2, D-ZK3, D-ZK79, D-LaK5, D-LaK6, D-LaK52, D-LaK70, D-ZF10, D-ZF93, D-LaF50, D-LaF050, D-LaF53, D-LaF79, D-ZLaF50, D-ZLaF52LA, D-ZLaF61, D-ZLaF67, D-ZLaF81, D-ZLaF85A,

D-ZLaF85L, H-QK3LGTi, H-K90GTi, QF50GTi, HWS1, HWS2, HWS3, HWS4, HWS5, HWS6, HWS7, HWS9, and HWS27.

The foregoing materials are the property of CDGM GLASS CO., LTD. For product information concerning these materials, see http://www.cdgmgd.com/. For other questions concerning the materials, please contact gmgd@cdgmgd.com.

Product catalog: www.cdgmglass.com/Glass-Finder

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S-LAH93,S-LAH95, S-LAH96, S-LAH97, S-LAH98, S-LAH99, S-FTM16, S-NBM51, S-NBH 5, S-NBH 8, S-NBH51, S-NBH52V, S-NBH53V, S-NBH55, S-NBH56, S-NBH57, S-NBH58, S-NPH 1, S-NPH 1W, S-NPH 2, S-NPH 3, S-NPH 4, S-NPH 5, S-NPH 7, L-BSL 7, L-BAL35, L-BAL35P, L-BAL42, L-BAL42P, L-BAL43, L-TIM28, L-TIM28P, L-LAL13, L-LAL15, L-LAM60, L-LAM69, L-LAH53, L-LAH84, L-LAH85V, L-LAH90, L-LAH91, L-LAH94, S-FPL51Y, S-FSL5Y, BSL7Y, BAL15Y, BAL35Y, BSM51Y, PBL1Y, PBL6Y, PBL25Y, PBL26Y, PBL35Y, PBM2Y, PBM8Y, PBM18Y, SK-1300, and SK-1310.

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3

# Ray Optics Interfaces

This chapter describes the physics interfaces found under the **Optics>Ray Optics** branch ( ).

In this chapter:

- The Geometrical Optics Interface
- Theory for the Geometrical Optics Interface

# The Geometrical Optics Interface

The **Geometrical Optics (gop)** interface ( ▯> ), found under the **Optics>Ray Optics**
branch ( ▯ ) when adding a physics interface, computes the paths of electromagnetic
waves in the high frequency limit. The wavefronts are treated as rays that can propagate
through optically large geometries and reflect or refract at boundaries. The
Geometrical Optics interface includes built-in options to compute the ray intensity,
polarization, phase, and optical path length. It is also fully compatible with deformed
geometries such as systems with thermal stress.

When this physics interface is added, these default nodes are also added to the **Model
Builder**: **Medium Properties**, **Material Discontinuity**, and **Ray Properties**. Then, from the
**Physics** toolbar, add other nodes that implement, for example, light sources or
boundary conditions. You can also right-click **Geometrical Optics** to select physics
features from the context menu.

## *Geometrical Optics Physics Interface Settings*

The **Label** is the physics interface name. The default is Geometrical Optics.

The **Name** is used primarily as a scope prefix for variables defined by the physics
interface. Refer to such physics interface variables in expressions using the pattern
<name>.<variable_name>. In order to distinguish between variables belonging to
different physics interfaces, the name string must be unique. Only letters, numbers, and
underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first physics interface in the model) is gop.

### RAY RELEASE AND PROPAGATION

The settings in this section affect the way in which primary and secondary rays are
released.

*Wavelength Distribution of Released Rays*
Select an option from the **Wavelength distribution of released rays** list: **Monochromatic**
(the default), **Polychromatic, specify vacuum wavelength**, or **Polychromatic, specify
frequency**.

- For **Monochromatic**, all rays in the model have the same vacuum wavelength and
  frequency, which is entered as a value or expression in the Ray Properties node.

- For **Polychromatic, specify vacuum wavelength**, a degree of freedom is allocated for the vacuum wavelength of each ray in the model. These degrees of freedom are initialized when the rays are released and are controlled by the **Vacuum Wavelength** section in the settings for the ray release features, such as Release from Grid.

- For **Polychromatic, specify frequency**, a degree of freedom is allocated for the frequency of each ray in the model. These degrees of freedom are initialized when the rays are released, and are controlled by the **Initial Ray Frequency** section in the settings for the ray release features, such as Release from Grid.

*Maximum Number of Secondary Rays*

The **Maximum number of secondary rays** limits the total number of secondary rays that can be created by capping them at the specified number. Secondary rays are released when an existing ray is subjected to certain boundary conditions. For example, when a ray arrives at a Material Discontinuity or Scattering Boundary between different media, the incident ray is refracted and a reflected ray is created; the degrees of freedom for this reflected ray are taken from one of the available secondary rays, which are preallocated when the study begins. Secondary rays are also used to model the interaction of rays with diffraction gratings, using the Grating boundary condition.

If an insufficient number of secondary rays are preallocated, a reflected ray may not be released when an existing ray undergoes refraction, even if some radiation should be reflected at the material discontinuity, and a warning message will be generated by the study. However, if a very large number of secondary rays are preallocated, then the number of degrees of freedom may become unnecessarily large. Thus, the **Maximum number of secondary rays** should only be large enough that all reflected rays which significantly affect the solution can be released. Rays that undergo total internal reflection at material discontinuities are not considered secondary rays and do not require extra preallocated degrees of freedom.

*Use Geometry Normals for Ray-Boundary Interactions*

By default the **Use geometry normals for ray-boundary interactions** check box is cleared. Then, whenever rays are reflected or refracted at boundaries, the surface normal is computed using the underlying mesh discretization of the boundary rather than the exact shape of the geometry itself. If this check box is selected, then the surface normal will instead be computed from an analytic representation of the geometry surfaces, if such an analytic representation can be obtained.

For the simple case of ray reflection by a parabolic edge in 2D, three example plots are shown in Figure 3-1 below. In the leftmost plot, linear geometry shape order has been specified; in other words, **Linear** has been selected from the **Geometry shape order** list

in the settings for the model component. The left figure also uses mesh normals. The reflected ray directions are visibly inaccurate because the boundary mesh is very coarse. The center figure uses **Linear** geometry shape order and geometry normals. Although the mesh is equally coarse, the reflected ray directions are much more accurate. The rightmost figure uses **Quadratic** shape order; because the edge is parabolic, this shape order results in reflected ray directions that are exact (to within machine precision) no matter whether mesh normals or geometry normals are used, because quadratic elements can perfectly represent a parabola.
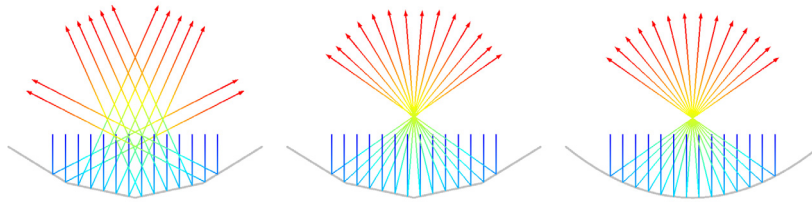


*Figure 3-1: Comparison of ray reflections at a parabolic boundary, using various definitions of the mesh normal.*

The **Use geometry normals for ray-boundary interactions** check box has no effect on the solution if the mesh can deform. This is true, for example, when the geometry is subjected to structural loads or thermal stresses. Then the mesh normal is always used.

*Only Store Accumulated Variables in Solution*

By default the **Only store accumulated variables in solution** check box is cleared. If this check box is selected, then the degrees of freedom associated with individual rays (such as the ray position, wave vector, intensity, power, and normalized Stokes parameters) will be solved for but not stored in the solution data. However, certain physics features define degrees of freedom in domains or on boundaries rather than on the individual rays, and these degrees of freedom will be retained in the solution. These quantities, called accumulated variables, are defined by the following features:

- Fluence Rate Calculation (domain)
- Deposited Ray Power (Domain)
- Deposited Ray Power (Boundary)
- Accumulator (Domain)
- Accumulator (Boundary)
- Nonlocal Accumulator (subnode to Release from Boundary)
- Ray Heat Source (multiphysics coupling)

It might be useful to discard ray degrees of freedom and only retain the accumulated variables when a very large number of rays are required to accurately solve for the accumulated variable. By only storing the accumulated variables, the file size can be significantly reduced.

While the **Only store accumulated variables in solution** check box is selected, if you run a study for the first time, the default **Ray** dataset and **Ray Trajectories** plot will not be created. If you later clear the check box and recompute the study, you may need to add these **Results** features manually.

---

▥     *Annular Ultraviolet Reactor*: Application Library path
**Ray_Optics_Module/Ultraviolet_Sterilization/annular_ultraviolet_reactor**

*Annular Ultraviolet Reactor with Particle Tracing*: Application Library path **Ray_Optics_Module/Ultraviolet_Sterilization/ annular_ultraviolet_reactor_particle**

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### MATERIAL PROPERTIES OF EXTERIOR AND UNMESHED DOMAINS

Use this section to control the properties of the void exterior to the model geometry as well as the properties of domains outside of the selection of the Geometrical Optics interface. For further details about what constitutes a "void" region, see the Geometry and Meshing section of the Ray Optics Modeling chapter.

*Optical dispersion model*

Select an option from the **Optical dispersion model** list: **Absolute vacuum**, **Specify refractive index** (the default), or **Air, Edlén (1953)**. This setting controls the refractive index in the empty space outside the geometry, called the void region. It also controls the refractive index for domains that are not included in the selection of the Geometrical Optics interface.

- For **Absolute vacuum**, the **Refractive index of exterior domains, real part** (dimensionless) is $n_{\text{ext}} = 1$. If ray power and/or intensity is being computed, the void region is assumed to be nonabsorbing.

- For **Specify refractive index**, enter a value or expression for the **Refractive index of exterior domains, real part.** The default is $n_{\text{ext}} = 1$. Enter a user defined value for **Refractive index of exterior domains, imaginary part** if power and/or intensity is being computed. The default is $k_{\text{ext}} = 0$.

- For **Air, Edlén (1953)**, the temperature and pressure dependent **Refractive index of exterior domains, real part** is computed using the model described in Ref. 2. The

model accepts user defined values of the **Exterior domain temperature** $T_{ext}$ (SI unit: K) and **Exterior domain pressure** $P_{ext}$ (SI unit: Pa). The defaults are $T_{ext} = 293.15$K and $P_{ext} = 1$ atm. See Optical Dispersion Models, The Refractive Index of Air for details.

For any type of optical dispersion model in the exterior and unmeshed domains, the algorithm to trace rays assumes that the medium is homogeneous. If a graded-index material is present, then its domain should be included in the selection of the Geometrical Optics interface and the spatial dependence of the refractive index should be controlled from the Medium Properties node.

### INTENSITY COMPUTATION

The settings in this section control the treatment of ray intensity and polarization. These settings are also important in multiphysics applications such as ray heating.

*Intensity Computation*

Select an option from the **Intensity computation** list: **None** (the default), **Compute intensity**, **Compute power**, **Compute intensity and power**, **Compute intensity in graded media**, or **Compute intensity and power in graded media**. For **None** no additional variables are computed along the rays. For other options, the ray intensity or ray power is computed as described below.

- For **Compute intensity**, auxiliary dependent variables are used to compute the intensity and polarization of each ray. For a complete list of the auxiliary dependent variables that are defined, see Intensity, Wavefront Curvature, and Polarization in Theory for the Geometrical Optics Interface. This option is only valid for computing intensity in homogeneous media; for graded-index media, use **Compute intensity in graded media** instead. The refractive index can still change discontinuously at boundaries, where the Fresnel equations are automatically used to compute the intensity of the reflected and refracted rays.

  The default name for the intensity variable is `gop.I`.

- For **Compute power**, the total power transmitted by each ray is defined as an auxiliary dependent variable. Information about the ray polarization is also available. The Deposited Ray Power (Boundary) subnode is available for the Wall feature. In addition, if a heat transfer interface such as the Heat Transfer in Solids interface is included in the model, the Ray Heat Source multiphysics node can be used to compute the heat source due to attenuation of rays within domains.

  The default name for the power variable is `gop.Q`.

- The option **Compute intensity and power** functions as a combination of the **Compute intensity** and **Compute power** options.

- The **Compute intensity in graded media** option functions like **Compute intensity** but is valid for both homogeneous and graded-index media. If all media in the model are homogeneous then it is recommended to select **Compute intensity** instead, since it is the more accurate method.

- The **Compute intensity and power in graded media** option functions like **Compute intensity and power** but is valid for both homogeneous and graded-index media. If all media in the model are homogeneous then it is recommended to select **Compute intensity and power** instead, since it is the more accurate method.

### Compute Phase

The **Compute phase** check box is only shown if the ray intensity is computed. Select the check box to allocate an auxiliary dependent variable for the phase of each ray. When the phase of each ray is computed, it is possible to plot interference patterns and visualize the instantaneous electric field components of polarized rays in postprocessing. When this check box is selected, the total number of degrees of freedom increases by 1 per ray. This option is based on the assumption that the coherence length of the radiation is arbitrarily large.

### Use Corrections for Strongly Absorbing Media

The **Use corrections for strongly absorbing media** check box is shown if the ray intensity is computed. Select the check box to accurately model reflection and refraction of rays at boundaries between strongly absorbing media, in which the imaginary part of the refractive index is very large. This option allocates two or three auxiliary dependent variables per ray based on space dimension. For more information about the way this option affects the intensity calculation, see Refraction in Strongly Absorbing Media in Theory for the Geometrical Optics Interface.

### Tolerance for Curvature Tensor Computation

When the **Intensity computation** is set to **Compute intensity in graded media** or **Compute intensity and power in graded media** enter a **Tolerance for curvature tensor computation** (dimensionless). This tolerance is used internally when computing the principal radii of curvature of propagating wavefronts in a graded medium. A larger tolerance makes the solution less accurate but more stable.

### ADDITIONAL VARIABLES

The options in this section can be used to solve for additional variables other than those that are used to compute intensity or define the ray frequency. By default, all of the check boxes in this section are cleared so that these variables are not solved for.

#### Compute Optical Path Length

Select the **Compute optical path length** check box to allocate an auxiliary dependent variable for the optical path length of each ray. The default variable name is gop.L. It is possible to reset the optical path length to 0 when rays interact with boundaries.

#### Count Reflections

Select the **Count reflections** check box to allocate an auxiliary dependent variable for the number of reflections undergone by each ray, including reflections by the Wall and Material Discontinuity features. The default variable name is gop.Nrefl. The auxiliary variable begins at 0 when rays are released and is incremented by 1 every time a ray is reflected at a boundary.

#### Store Ray Status Data

Select the **Store ray status data** check box to add new variables for quantities that cannot necessarily be recovered from the ray trajectory data alone. This is especially true if automatic remeshing is used in a model. The variables created include the following, all of which would be preceded by the physics interface tag (for example, gop.):

- The release time of a given ray (variable name rti).
- The time at which a ray stopped at a boundary (variable name st).
- The final status of the ray (variable name fs). This indicates the status of a ray at the final time step. The value is an integer which has one of the following values:
  - 0 for unreleased rays
  - 1 for rays that are still in the modeling domain
  - 2 for frozen rays
  - 3 for stuck rays
  - 4 for rays that have disappeared

To summarize the total number of rays having each final status, the following global variables are also defined.

TABLE 3-1:  GLOBAL VARIABLES BASED ON RAY STATUS

| NAME | DESCRIPTION |
|------|-------------|
| fac | Fraction of active rays at final time step |
| fds | Fraction of disappeared rays at final time step |
| ffr | Fraction of frozen rays at final time step |
| fse | Fraction of secondary rays released |
| fst | Fraction of stuck rays at final time step |
| nsr | Number of released secondary rays |
| nsrf | Number of released secondary rays at final time step |
| nsu | Number of unreleased secondary rays |
| nsuf | Number of unreleased secondary rays at final time step |

The global variable names in Table 3-1 all take the unreleased secondary rays into account. For example, suppose an instance of the Geometrical Optics interface includes 100 primary rays and 100 allocated secondary rays. At the last time step, suppose that 80 of the primary rays have disappeared at boundaries and that 40 secondary rays have been emitted, all of which are still active. Then the variable gop.fac, the fraction of active rays at the final time step, would have the value $(20 + 40)/(100 + 100)$ or 0.3.

**ADVANCED SETTINGS**

This section is only shown when **Advanced Physics Options** are enabled (click the **Show More Options** button  in the **Model Builder** toolbar, and select **Advanced Physics Options** in the **Show More Options** dialog box). These options are hidden by default because it is only necessary to modify them under very specific circumstances.

*Wall Accuracy Order*

The **Wall accuracy order** sets the accuracy order of the time stepping used for time steps during which a ray-wall interaction happens. Select an order of **1** to use a forward Euler step and compute the direction or ray propagation both before and after the wall interaction. Select an order of **2** (the default) to use a second-order Taylor method to compute the trajectory before the wall interaction. After the ray-wall interaction a second-order Runge-Kutta method is used. Usually this setting has no effect on the ray tracing calculation because the rays move along straight lines, but the higher wall accuracy order is more accurate if graded-index media are present.

*Arguments for Random Number Generation*

Select an option from the **Arguments for random number generation** list: **Generate unique arguments** (the default), **Generate random arguments**, or **User defined**. This setting determines how the additional argument to the `random` function is defined in features such as the Wall boundary condition with the **Diffuse scattering** wall condition. Typically the random numbers are functions of the ray index, time, a unique input argument for different variable definitions, and another argument $i$, defined as follows:

- For **Generate unique arguments** the additional argument is based on the position of each node in the Model Builder. As a result, random numbers generated in different nodes are created independently of each other.

- For **Generate random arguments** the additional argument is randomly created each time the study is run.

- For **User defined** the additional argument is defined by a user input in the **Settings** window for each feature. Uncorrelated sets of random numbers can be obtained by running a **Parametric Sweep** for different values of $i$.

Note that the `random` function is a pseudorandom number generator (PRNG), not a true random number generator (RNG) in the sense that an observer with perfect knowledge of the algorithm and a history of previously generated values could predict the ensuing values. However, PRNG is sufficient for most purposes.

For any model using PRNG, it is recommended to test for statistical convergence by varying the number of rays and observing the effect on some ray statistics, such as average final ray position or transmission probability. This is analogous to the mesh refinement studies that are typically recommended to validate finite element models.

*Allow Multiple Release Times*

The **Allow multiple release times** check box, which is cleared by default, allows an array of release times for the rays to be specified in any of the ray release features. If the check box is cleared, all rays are released at time $t = 0$.

*Exclude Jacobian Contributions from Ray Equations*

By default the **Exclude Jacobian contributions from ray equations** check box is cleared. If this check box is selected, then expressions for the time derivatives of the degrees of freedom on rays are not included in the Jacobian matrix. Excluding contributions to the Jacobian can significantly improve solution time if the number of rays in the model is very large. The drawback is that the Jacobian is not exact, so smaller time steps or path length intervals may be needed to obtain an accurate solution. This drawback is most noticeable when computing the ray intensity or power in an absorbing medium.

*Treat Unmeshed Releasing Entities as Errors*

By default the **Treat unmeshed releasing entities as errors** check box is selected. Certain ray release features, such as the **Release** and **Release from Boundary** features, compute the ray release positions based on a geometric entity, which must be meshed. While this check box is selected, failure to mesh the selections of such features will result in an error message when running any study in the model. If this check box is cleared, failure to mesh the selections of such features will result in them releasing zero rays, but will otherwise not interrupt the computation. Other physics features will still be able to release rays normally.

*Maximum Number of Wall Interactions per Time Step*

Enter a value for the **Maximum number of wall interactions per time step**. The default value is 1000. If a ray undergoes more than the specified number of boundary interactions in a single time step taken by the solver, the ray will disappear. This is included as a safeguard to prevent rays from getting stuck in infinite loops if the time between successive ray-wall interactions becomes infinitesimally small.

### DEPENDENT VARIABLES

The dependent variables (field variables) are the components of the **Ray position** and **Wave vector.** The name can be changed but the names of fields and dependent variables must be unique within a model. In 3D, the default ray position vector components are qx, qy, and qz; and the default wave vector components are kx, ky, and kz.

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| | |
|---|---|
| 🔍 | [Theory for the Geometrical Optics Interface](#) |

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## *List of Geometrical Optics Interface Physics Features*

[The Geometrical Optics Interface](#) has the following nodes and subnodes (listed in alphabetical order) available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

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| | |
|---|---|
| 💡 | In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu. |

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- Accumulator (Boundary)
- Accumulator (Domain)
- Auxiliary Dependent Variable
- Axial Symmetry
- Blackbody Radiation
- Circular Wave Retarder
- Cross Grating
- Deposited Ray Power (Boundary)
- Deposited Ray Power (Domain)
- Diffraction Order (Grating)
- Diffraction Order (Cross Grating)
- Fluence Rate Calculation
- Gaussian Beam
- Grating
- Ideal Depolarizer
- Ideal Lens
- Illuminated Surface
- Linear Polarizer
- Linear Wave Retarder
- Material Discontinuity
- Medium Properties
- Mirror
- Mueller Matrix

- Nonlocal Accumulator
- Photometric Data Import
- Ray Continuity
- Ray Detector
- Ray Properties
- Ray Termination
- Release
- Release from Data File
- Release from Boundary
- Release from Edge
- Release from Electric Field
- Release from Far-Field Radiation Pattern
- Release from Grid
- Release from Grid on Axis
- Release from Point
- Release from Point on Axis
- Release from Symmetry Axis
- Scattering Domain
- Scattering Boundary
- Solar Radiation
- Thin Dielectric Film
- Wall

## Ray Properties

The **Ray Properties** node is added by default. Only one instance of this node can exist for each physics interface. The **Ray Properties** node defines the equations for ray propagation and may also include inputs for some ray properties.

**RAY PROPERTIES**
This section is shown when **Monochromatic** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section.

Otherwise the frequency or vacuum wavelength of released rays is controlled separately by each ray release feature, such as Release or Release from Grid.

Select an option from the **Ray property specification** list: **Specify vacuum wavelength** (the default) or **Specify frequency**.

- For **Specify vacuum wavelength** enter a **Vacuum wavelength** $\lambda_0$ (SI unit: m). The default is 660 nm.

- For **Specify frequency** enter a **Ray frequency** $v$ (SI unit: Hz). The default is $4.54 \times 10^{14}$ Hz.

## *Medium Properties*

Use the **Medium Properties** node to specify the refractive index of the medium. An instance of this feature is created by default, including all of the selected domains for the physics interface. For the region outside the geometry and for any domains not included in the physics interface selection, the refractive index is instead controlled by the **Optical dispersion model** in the physics interface **Material Properties of Exterior and Unmeshed Domains** section.

### MEDIUM PROPERTIES

Use the settings in this section to specify how the real part of the refractive index is defined. If the ray intensity or power is computed, then you can also specify the imaginary part of the refractive index, which is used to describe absorption within the medium.

*Refractive Index of Domains*

Choose an option from the **Refractive index of domains** list:

- If **Specify absolute refractive index** (the default) is selected, the **Refractive index, real part** can be taken **From material**, or it can be entered directly. The default value is 1. This index is considered absolute, that is, relative to vacuum.

- If **Specify relative refractive index** is selected, the **Refractive index, real part** can be taken **From material**, or it can be entered directly. The default value is 1. Then enter the **Reference temperature** $T_{\mathrm{ref,rel}}$ (SI unit: K, default 293.15 K) and the **Reference pressure** $P_{\mathrm{ref,rel}}$ (SI unit: Pa, default 0). The given refractive index is understood to be relative to air; that is, the absolute refractive index is the product of the specified value with the refractive index of air at the reference temperature and pressure.

- If **Get dispersion model from list** is selected, choose an option from the **Optical dispersion model** list. The following options are available:

  - **Cauchy**,
  - **Conrady**,
  - **Herzberger**,
  - **Schott**,
  - **Schott extended**,
  - **Sellmeier**,
  - **Sellmeier modified, type 1**,
  - **Sellmeier modified, type 2**, and
  - **Temperature-dependent Sellmeier**.

- If **Get dispersion model from material** is selected, the dispersion model in each domain is automatically deduced from the **Material** nodes and their selections. This allows different optical dispersion models to be used in different domains in the geometry, using only a single **Medium Properties** node.

  For example, suppose that a model contains two lenses consisting of two different glasses, and that the first glass is defined using **Sellmeier** coefficients whereas the second glass is defined using **Schott** coefficients. Then selecting **Get dispersion model from material** will automatically express the refractive index using the **Sellmeier** equation in the first lens and the **Schott** (polynomial) equation in the second. An alternative way to use different optical dispersion models in different domains is to use more than one instance of the **Medium Properties** node and select the dispersion models manually.

  For more information on each optical dispersion model, see Table 3-3 in Theory for the Geometrical Optics Interface, Optical Dispersion Models section.

  The coefficients for each of these dispersion models are taken **From material** by default. Alternatively, **User defined** coefficients may be entered.

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| ! | For the built-in optical dispersion models, the wavelength is always assumed to be in units of microns (μm). For example, in the **Schott** (polynomial) model, the coefficients $A_0, A_1, A_2, A_3$, and so on have units of $1$, μm, $\mu m^2$, $\mu m^3$, and so on. If another source were to provide these coefficients using nanometers instead of microns, then some manual conversion would be required. |
|---|---|

Similar to the option **Specify relative refractive index**, most of the built-in optical dispersion models define the refractive index relative to air, and therefore they all require a reference temperature and pressure to be specified. The only exception is the **Temperature-dependent Sellmeier**, in which the refractive index is assumed to be absolute, such that $n = 1$ is the refractive index of an ideal vacuum. To use any other optical dispersion model to define an absolute index, set the reference pressure to zero.

Using the **Temperature-dependent Sellmeier** model also disables the settings for selecting a **Thermo-optic dispersion model** (see the following subsection).

The conversion from relative to absolute refractive index is made using the Edlén model (Ref. 2) for the refractive index of air. See Optical Dispersion Models for further details.

*Optical Attenuation Model*
By default the **Optical attenuation model** list is not shown. However, it will be shown if you select any option except **None** from the **Intensity computation** list in the physics interface settings. This is because the speed of light in a medium only depends on the real part of the refractive index, whereas the imaginary part affects the attenuation of ray intensity or power if they are solved for.

The standard used by the Geometrical Optics interface is to treat absorbing media as having complex-valued refractive indices of the form $n - i\kappa$, where $n$ and $\kappa$ are real dimensionless numbers and $\kappa > 0$. The case $\kappa < 0$ would constitute a gain medium.

The **Optical attenuation model** list has the following options:

- For **Extinction coefficient**, specify the value of $\kappa$ directly. This can be taken **From material** or **User defined**; if **User defined** the default is 0. The Geometrical Optics interface only recognizes isotropic $\kappa$ where the absorption rate does not depend on ray polarization.

- For **Attenuation coefficient**, specify the value of the **Attenuation coefficient** $\alpha$ (SI unit: 1/m) which is related to $\kappa$ by $\alpha = 4\pi\kappa/\lambda_0$. The default is 1 1/m.

- For **Internal transmittance, 2 mm sample thickness**, enter a value or expression for the internal transmittance of a 2 mm thick sample of the material, neglecting Fresnel losses. Internal transmittances are dimensionless and are denoted $\tau_{i,d}$, where $d$ is replaced with the sample thickness, for example, $\tau_{i,2}$. The default is 0.9. The relationship between $\tau_{i,d}$ and $\kappa$ is $\kappa = -(\lambda_0 \log \tau_{i,d})/(4\pi d)$.

- The remaining options are internal transmittances at other values of the sample thickness. Options for 5 mm, 10 mm, and 25 mm samples are available. Otherwise the settings are the same as the **Internal transmittance, 2 mm sample thickness** option.

*Conversions Between Optical Attenuation Models*

The material properties for different optical attenuation models are used to define the corresponding properties for other attenuation models automatically. For example, if you select **Extinction coefficient** and try to take the value of κ **From material**, but the selected material only has internal transmittance data, then the value of the internal transmittance data is automatically converted to a value of κ based on the wavelength.

If the selected material has internal transmittance data for two or more sample thicknesses, the data for the greatest thickness is automatically used unless otherwise specified. This default behavior is intended to give the best possible numerical precision when the internal transmittance values are close to 1, implying weak absorption. However, it may be preferable to use internal transmittance data for a smaller sample thickness in IR or UV applications when most of the energy is absorbed.

*How to Automatically Detect Optical Dispersion Models*

The option **Get dispersion model from material** is unique because it allows a single **Medium Properties** node to detect different optical dispersion models from a large number of different materials having different domain selections. For example, the materials used in the Petzval Lens tutorial are shown in Figure 3-2 below. To automatically detect the optical dispersion models of the loaded glasses, take the following steps:

**1** Add materials to the model using the Optical Material Library. Most of the glasses in this material library use an optical dispersion model to define the refractive index. As the materials are added, the coefficients used by the optical dispersion model are automatically loaded.

**2** Locate the default **Medium Properties** node.

**3** From the **Refractive index of domains** list, select **Get dispersion model from material**. If the glasses loaded in step 1 also provide thermo-optic coefficients, it is important to specify an accurate value of the **Temperature** as well.
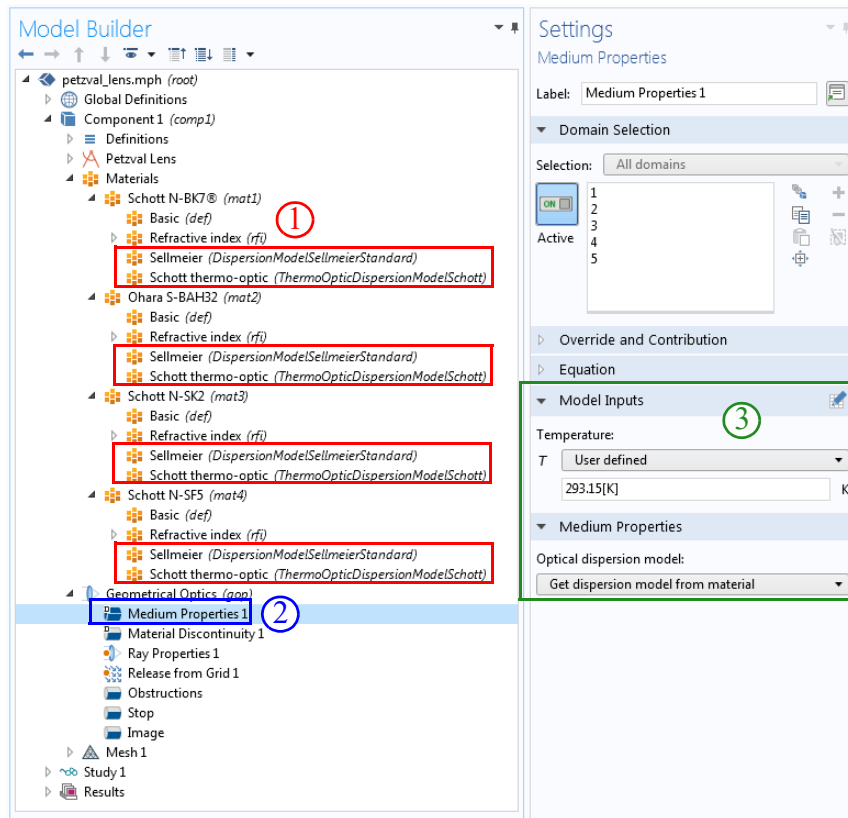
*Figure 3-2: Workflow for automatically detecting optical dispersion models from the glasses in an optical prescription.*

### Thermo-Optic Dispersion Models

A temperature-dependent offset in the Refractive index may be specified using a thermo-optic dispersion model. Two options are possible:

- **None** (the default): no offset will be applied.
- **Schott thermo-optic**: this is the only built-in thermo-optic dispersion model available. The coefficients used to compute a temperature dependent offset in the refractive index can either be taken **From material** (the default), or **User defined**. A reference temperature is also required. This may also be taken **From material** (the default), or **User defined**.

For further details, see Thermo-Optic Dispersion Models.

*Material Discontinuity*

The **Material Discontinuity** node is the default feature on all boundaries.

The Geometrical Optics interface always applies reflection and refraction at boundaries between different media using a deterministic ray splitting approach. The direction of the refracted ray is computed using Snell's law, based on the refractive index on either side. If extra degrees of freedom have been allocated for secondary rays, a reflected ray is also released. If the incident ray undergoes total internal reflection, no refracted ray is produced and no secondary rays are needed to release the reflected ray.

You can use the **Rays to Release** section (see below) to decide whether to split the incident ray into reflected and refracted rays, or to ignore the reflected ray.

If the ray intensity or power is solved for in the model, the **Material Discontinuity** feature computes the new values of these variables for the reflected and refracted rays. This reinitialization uses the Fresnel Equations while accounting for the incident ray polarization and the influence of any dielectric films on the surface reflectance.

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| 📑 | The maximum number of reflected rays can be controlled via the **Maximum number of secondary rays** text field, which is found under the **Ray Release and Propagation** section for the physics interface. |
| | If a reflected ray should be produced, but all of the preallocated secondary rays have already been released, the study will produce a **Warning** node. |

The Accumulator (Boundary) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. The Thin Dielectric Film subnode is also available if the following conditions are met:

• The ray intensity or power is being computed, and
• One of the following options is selected from the **Thin dielectric films on boundary** list in the **Coatings** section: **Add layers to surface** or **Add layers to surface, repeating**.

**COATINGS**

This section is available if ray intensity or power is being computed in the model. Use the options in this section to add thin dielectric layers to the boundary between the media. These thin dielectric layers are used, together with the refractive indices on either side, to modify the Fresnel equations for the reflection and transmission coefficients at the boundary.

The thicknesses of the thin dielectric layers must be small relative to the coherence length of the radiation. They are usually comparable in length scale to the free-space wavelength.

Select an option from the **Thin dielectric films on boundary** list. The default is **None**. The following options are available.

- **None**: no dielectric films are on the boundary. The intensity of the reflected and refracted light is computed solely using the Fresnel equations with the refractive indices of the two adjacent domains.

- **Add layers to surface**: you can add any number of thin dielectric films to the boundary by adding one or more Thin Dielectric Film subnodes; right click the **Material Discontinuity** node or select **Thin Dielectric Film** from the **Physics** toolbar, **Attributes** menu. If multiple thin films are added to a single surface, they are arranged in the same order as the corresponding **Thin Dielectric Film** subnodes in the Model Builder, from the upside of the boundary toward the downside.

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| ⊞ | *Anti-Reflective Coating with Multiple Layers*: Application Library path **Ray_Optics_Module/Prisms_and_Coatings/antireflective_coating_multilayer** |

- **Add layers to surface, repeating**: this option functions like the **Add layers to surface** option described above. Add individual dielectric coatings to the boundary using the **Thin Dielectric Film** subnode. In addition, enter a value or expression for the **Number of repeating unit cells** $N$ (dimensionless). The default value is $3$. In the settings windows for the **Thin Dielectric Film** subnodes, you can decide which layers constitute a unit cell that will be repeated the specified number of times. Use this option to specify periodic arrangements with a large number of repeatind dielectric layers, without having to add each layer manually.

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| ⊞ | *Distributed Bragg Reflector*: Application Library path **Ray_Optics_Module/Prisms_and_Coatings/distributed_bragg_reflector** |

- **Anti-reflective coating**: the incident ray is refracted with unit transmittance and zero reflectance.

- **Single-layer coating, specified thickness**: this is a simplified version of the **Add layers to surface** option that only allows a single dielectric layer. Enter a value or expression for the **Film refractive index** $n$ (dimensionless). The default value is $1$. Then enter a value or expression for the **Film thickness** $t$ (SI unit: m). The default value is $1 \, \mu m$.

- **Specify reflectance**: enter a value or expression for the reflectance at the boundary directly. Enter a value or expression for the **Reflectance $R$** (dimensionless). The default is $0.1$. If the **Specify different values for s- and p-polarization** check box is selected, you can instead enter separate values for the reflectance of p- and s-polarized light, called $R_p$ and $R_s$, respectively. The layers are considered nonabsorbing so that the sum of the reflectance and transmittance is unity.

- **Specify transmittance**: enter a value or expression for the transmittance at the boundary directly. Enter a value or expression for the **Transmittance $T$** (dimensionless). The default is $0.9$. If the **Specify different values for s- and p-polarization** check box is selected, you can instead enter separate values for the transmittance of p- and s-polarized light, called $T_p$ and $T_s$, respectively. The layers are considered nonabsorbing so that the sum of the reflectance and transmittance is unity.

*Real and Ideal Optical Coatings*

The options **Anti-reflective coating**, **Specify reflectance**, and **Specify transmittance** all include a check box called **Treat as single layer dielectric film**, which is cleared by default. While this check box is cleared, the specified reflectance or transmittance applies to all rays, regardless of wavelength or angle of incidence, and the remaining inputs in this section are not shown. This makes complicated multilayer films easier to set up because you can enter the reflectance or transmittance explicitly without having to know the properties of each layer in the coating. If the coating properties depend on the wavelength or angle of incidence, you can usually build this dependence into the model by defining the film reflectance or transmittance as an **Interpolation** function of the ray properties. The tradeoff is that accurate information about the discontinuities in ray phase is lost, even if the **Compute phase** check box is selected in the physics interface **Intensity Computation** section, because this information depends on the complex-valued Fresnel coefficients.

If the **Treat as single layer dielectric film** check box is selected, then instead the **Material Discontinuity** automatically computes the thickness of a single layer needed to produce the given reflectance or transmittance. The drawback is that the specified value will only be attained for rays at a specific wavelength and angle of incidence.

The following inputs are only shown when **Treat as single layer dielectric film** is selected.

For **Specify reflectance** and **Specify transmittance** enter the **Film refractive index $n$** (dimensionless). The default is $1$. If it is impossible to construct a single layer of this refractive index and obtain the specified reflectance or transmittance, then the boundary is treated as having no dielectric films. For **Anti-reflective coating**, the

refractive index of the coating is not an input because it is always the geometric mean of the refractive indices in the two adjacent domains.

For **Anti-reflective coating**, **Specify reflectance**, and **Specify transmittance** enter the following:

- **Vacuum wavelength for specified film properties** $\lambda_0$ (SI unit: m). The default is 660 nm.

- **Angle of incidence for specified film properties** $\theta_i$ (SI unit: m). The default is $0$.

- Select an option from the **Angle of incidence specification** list: **With respect to upside** (the default) or **With respect to downside**. You can see which side is the upside by selecting the **Show boundary normal** check box (see **Advanced Settings** below); the normal vector rendered in the Graphics window points from the upside to the downside.

- Select an option from the **Specified film behavior applies to** list: **S-polarized radiation** (the default) or **P-polarized radiation**.

### RAYS TO RELEASE

Use the inputs in this section to control whether the incident ray is split into a reflected and refracted ray at the material discontinuity. Select an option from the **Release reflected rays** list: **Always** (the default), **Never**, or **Based on logical expression**.

- If **Always** is selected, whenever a ray hits the material discontinuity, the incident ray is refracted across the boundary, and a reflected ray is produces using some of the preallocated degrees of freedom for secondary rays.

- If **Never** is selected, the incident ray is refracted, but no reflected ray is produced. This does not prevent a ray from undergoing total internal reflection at the boundary.

- If **Based on logical expression** is selected, enter a value or expression for the **Evaluation expression** $e$ (dimensionless). The default is $1$. A reflected ray is produced only if the value of this expression is nonzero for the incident ray.

If the ray intensity is solved for in the model, enter a **Threshold intensity** $I_{th}$ (SI unit: W/m$^2$). The default is $1$ mW/m$^2$. If the interaction of a ray with a material discontinuity would create a reflected ray of intensity less than the threshold intensity, the release of this reflected ray is suppressed.

If the ray power is solved for in the model, enter a **Threshold power** $Q_{th}$ (SI unit: W). The default is $10^{-3}$ mW. If the interaction of a ray with a material discontinuity would create a reflected ray of power less than the threshold power, the release of this

reflected ray is suppressed. Suppressing the release of reflected rays of extremely low intensity or power is a convenient way to avoid wasting computational resources.

If both the **Evaluation expression** and the **Threshold intensity** are specified, a reflected ray is only released if the value of the expression is nonzero and the intensity of the reflected ray exceeds the threshold. In other words, a ray must satisfy all of the criteria in the **Rays to Release** section in order to be released, not just one of them.

### AUXILIARY DEPENDENT VARIABLES, REFRACTED RAY

This section includes a check box (cleared by default) and a text field (default 0) for every Auxiliary Dependent Variable in the model. Select the check box to activate the text field, which controls the new value of this auxiliary dependent variable for the refracted ray. If the check box is cleared, the new value equals that of the incident ray.

The value can be a function of any combinations of ray variables and variables defined on the boundary. For example, to increment the value of psi by 1 when a ray touches or crosses a boundary, enter psi+1 in the text field for $psi_{new}$.

### AUXILIARY DEPENDENT VARIABLES, REFLECTED RAY

This section is the same as Auxiliary Dependent Variables, Refracted Ray, except that the expressions are used to auxiliary dependent variables for the reflected ray.

### ADVANCED SETTINGS

Select the **Show boundary normal** check box to view the boundary normal in the **Graphics** window.

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| **!** | Visualization of the boundary normal is important when adding multiple Thin Dielectric Film subnodes, since the thin films are oriented from the upside of the boundary to the downside in the same order as their corresponding nodes in the Model Builder. |

If the **Compute optical path length** check box is selected in the physics interface **Additional Variables** section, select the **Reset optical path length** check box to set the optical path length of reflected and refracted rays to 0. Otherwise both the reflected and refracted ray inherit the optical path length of the incident ray.

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| **Q** | Material Discontinuity Theory |

*Thin Dielectric Film*

Use the **Thin Dielectric Film** subnode to model the interaction of rays with walls or material discontinuities that are coated with thin, transparent dielectric layers. The presence of these layers modifies the Fresnel coefficients used to compute the intensity or power of the reflected and refracted rays. The films must be very thin relative to the coherence length of the radiation and are usually comparable to or smaller than the wavelength. The subnode is available from the context menu (right-click the Material Discontinuity or Wall parent node) or from the **Physics** toolbar, **Attributes** menu.

The **Thin Dielectric Film** subnode is applied to all boundaries in the selection of the **Wall** or **Material Discontinuity** parent node. The effects of the **Thin Dielectric Film** subnodes are applied when computing the coefficients of reflection and transmission, which are necessary for the reinitialization of Stokes parameters during reflection and refraction if the intensity is solved for in the model.

### FILM PROPERTIES

Enter a **Film refractive index** $n$ (dimensionless). The default value is $1$. Then enter a **Film thickness** $t$ (SI unit: m). The default is $1\ \mu m$.

### REPEATING MULTILAYER FILMS

If **Add layers to surface, repeating** is selected from the **Thin dielectric films on boundary** list in the **Coatings** section in the settings window for the parent node, this section is used to determine which layers are part of the repeating unit cell of a periodic multilayer film. If the **Repeat layer in multilayer films** check box is selected, the layer is repeated a number of times equal to the **Number of repeating unit cells** specified in the parent node settings window. If the check box is cleared, the layer will appear only once in multilayer films.

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🔍　　　Thin Dielectric Film Theory

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*Wall*

Use the **Wall** node to determine what happens to the rays when contact with a boundary is made. Rays automatically detect walls that intersect their path, without the order of the interactions being specified. At boundaries, rays can be reflected or absorbed. You can also select two different conditions and assign a criterion or probability to determine which one is applied.

The Accumulator (Boundary) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu. If the ray intensity or power is computed, the Thin Dielectric Film subnode is also available. If the ray power is computed, the Deposited Ray Power (Boundary) subnode is also available.

**WALL CONDITION**

Select a **Wall condition**: **Freeze** (the default), **Specular Reflection**, **Stick**, **Disappear**, **Pass through**, **Diffuse scattering**, **Isotropic scattering**, **Mixed diffuse and specular reflection**, or **General reflection**.

TABLE 3-2: WALL CONDITION OPTIONS

| OPTIONS | DESCRIPTION |
|---|---|
| Freeze | Select to fix the ray position and wave vector at the instant a wall is struck. So, the ray position no longer changes after contact with the wall and the wave vector of the ray remains at the same value as when the ray struck the wall. This boundary condition is typically used to recover the ray intensity or phase at the instant contact was made with the wall. |
| Specular Reflection | Select to specularly reflect from the wall, so that the angle of incidence and the angle of reflection are equal. |
| Stick | Select to fix the ray position at the instant the wall is struck. The wave vector components are set to zero. |
| Disappear | This option means that the ray is not displayed once it has made contact with the wall. Use it if the ray location after contact with the wall is not of interest. |
| Pass through | This option allows rays to cross the boundary unimpeded. It does not change the ray direction at a boundary between different media; to model refraction, instead use the Material Discontinuity feature. |
| Diffuse scattering | Select to reflect rays at a wall according to Lambert's cosine law. That is, the probability of a reflected ray propagating in a given direction within a solid angle $d\omega$ is given by $\cos(\theta)d\omega$ where $\theta$ is the angle between the direction of the ray and the wall normal. |
| Isotropic scattering | Select to reflect rays at a wall isotropically in random directions. |
| Mixed diffuse and specular reflection | Select to reflect rays at a wall either specularly or according to Lambert's cosine law, based on a user-defined probability. |
| General reflection | Select to allow an arbitrary direction vector to be specified after a ray makes contact with the wall. The ray direction vector components can be functions of the incident ray direction, phase, or any other quantity. |

This section is available when **General reflection** (see Table 3-2) is selected as the **Wall condition**.

Enter values for the **Reflected ray direction vector** $\mathbf{L}_p$ (dimensionless) either in Cartesian coordinates $(x, y, z)$ (the default) or select the **Specify tangential and normal direction vector components** check box to enter coordinates in the tangent-normal coordinate system $(t_1, t_2, n)$. In this case the normal direction is selected so that an incident ray is reflected back into the domain it previously occupied if the specified normal direction vector component is positive. The tangential directions are oriented so that they form a right-handed coordinate system, together with the normal direction.

**PRIMARY RAY CONDITION**

Use this section to apply two different wall conditions on the same set of boundaries based on a probability or logical expression.

Select a **Primary ray condition**: **None** (the default), **Probability**, or **Expression**. When the default, **None**, is kept, it means that the **Wall condition** is always respected by the incident rays.

*Probability*
If **Probability** is selected, the **Wall condition** is applied with a certain probability. Enter a value for the **Probability**, $\gamma$ (dimensionless). If the **Wall condition** is not used, the ray instead behaves according to the **Otherwise** setting.

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📑      The value of $\gamma$ should always be between 0 and 1.

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For example, if the **Wall condition** is set to:

- **Freeze** and $\gamma$ is set to 0.1, then for every 10 rays that strike the wall, on average one freezes and the remaining 9 rays behave according to the **Otherwise** setting.
- **Stick** and $\gamma$ is set to 0.5 then on average half of the rays stick to the wall and the other half behave according to the **Otherwise** setting.

*Expression*
If **Expression** is selected, the **Evaluation expression** $e$ (dimensionless) is evaluated whenever a ray strikes the wall. The default expression is 1. If the Evaluation expression is nonzero, the ray behaves according to the **Wall condition**, otherwise the ray behaves according to the **Otherwise** setting.

*Otherwise*

The options available for the **Otherwise** setting are the same as for the **Wall Condition**, except that **General reflection** and **Mixed diffuse and specular reflection** are not available. The **Otherwise** setting can be used to make rays interact with a wall differently with a certain probability or when a certain condition is satisfied. For example, to model reflection at a partially specular surface in which 50% of the ray intensity is absorbed and 30% is reflected specularly:

- Select **Mixed diffuse and specular reflection** as the **Wall condition**,

- set the **Probability of specular reflection** to 0.3/(1-0.5),

- set the **Primary ray condition** to **Probability**,

- set the **Probability** to 1-0.5, and

- select **Freeze** as the **Otherwise** option.

### FREQUENCY REINITIALIZATION

This section is available when **Polychromatic, specify frequency** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section, and when a **Wall Condition** (or **Otherwise** condition) other than **Freeze**, **Stick**, or **Disappear** is selected.

This section allows the ray frequency to be changed when rays are reflected by the boundary or pass through it. To do so, select the **Reinitialize frequency** check box; it is cleared by default. Then select one of the following from the **Distribution function** list:

- **None** (the default): enter a value or expression for the Ray frequency $\nu$ (SI unit: Hz) directly. The default is $3 \times 10^{14}$ Hz.

- **Normal**: the new value of the ray frequency is sampled from a normal or Gaussian distribution. Enter a value or expression for the **Mean ray frequency** $\mu$ (SI unit: Hz). The default is $3 \times 10^{14}$ Hz. Then enter a value or expression for the **Ray frequency standard deviation** $\sigma$ (SI unit: Hz). The default is $3 \times 10^{13}$ Hz.

- **Lognormal**: the new value of the ray frequency is sampled from a lognormal distribution; that is, its logarithm follows a normal or Gaussian distribution. A big advantage of the **Lognormal** distribution (compared to the **Normal** distribution) is that it statistical outliers will never cause the frequency to become negative. Enter a value or expression for the **Mean ray frequency** $\mu$ (SI unit: Hz). The default is

$3 \times 10^{14}$ Hz. Then enter a value or expression for the **Ray frequency standard deviation** $\sigma$ (SI unit: Hz). The default is $3 \times 10^{13}$ Hz.

- **Uniform**: the new value of the ray frequency will be sampled uniformly from an interval. Enter a value or expression for the **Minimum ray frequency** $\nu_{min}$ (SI unit: Hz). The default is $3 \times 10^{14}$ Hz. Then, enter a value or expression for the **Maximum ray frequency** $\nu_{max}$ (SI unit: Hz). The default is $3.5 \times 10^{14}$ Hz.

**WAVELENGTH REINITIALIZATION**

This section is available when **Polychromatic, specify vacuum wavelength** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section, and when a **Wall Condition** (or **Otherwise** condition) other than **Freeze**, **Stick**, or **Disappear** is selected.

This section allows the wavelength to be changed when rays are reflected by the boundary or pass through it. To do so, select the **Reinitialize wavelength** check box; it is cleared by default. Then select one of the following from the **Distribution function** list:

- **None** (the default): enter a value or expression for the **Vacuum wavelength** $\lambda_0$ (SI unit: Hz) directly. The default is 500 nm.
- **Normal**: the new value of the wavelength is sampled from a normal or Gaussian distribution. Enter a value or expression for the **Mean vacuum wavelength** $\mu$ (SI unit: m). The default is 500 nm. Then enter a value or expression for the **Vacuum wavelength standard deviation** $\sigma$ (SI unit: m). The default is 50 nm.
- **Lognormal**: the new value of the wavelength is sampled from a lognormal distribution; that is, its logarithm follows a normal or Gaussian distribution. A big advantage of the **Lognormal** distribution (compared to the **Normal** distribution) is that it statistical outliers will never cause the wavelength to become negative. Enter a value or expression for the **Mean vacuum wavelength** $\mu$ (SI unit: m). The default is 500 nm. Then enter a value or expression for the **Vacuum wavelength standard deviation** $\sigma$ (SI unit: m). The default is 50 nm.
- **Uniform**: the new value of the wavelength will be sampled uniformly from an interval. Enter a value or expression for the **Minimum vacuum wavelength** $\lambda_{0,min}$ (SI unit: m). The default is 500 nm. Then, enter a value or expression for the **Maximum vacuum wavelength** $\lambda_{0,max}$ (SI unit: m). The default is 550 nm.

**ABSORPTION COEFFICIENT**

This section is available when

- the ray intensity or power is solved for in the model, and

- the **Wall condition** is set to any option that can reflect rays, including the following:

    - **Specular Reflection**,

    - **Diffuse scattering**,

    - **Isotropic scattering**,

    - **General reflection**, or

    - **Mixed diffuse and specular reflection**.

Select one of the following from the **Compute reflected intensity using** list: **Absorption coefficients** or **Reflection coefficients**.

For **Absorption coefficients** enter the **Absorption coefficient** $\alpha$ (dimensionless). The default is $0$. The intensity or power of the reflected ray will be proportional to $1 - \alpha$.

For **Reflection coefficients** enter the **Reflection coefficient** $r$ (dimensionless). The default value is $1$. The intensity or power of the reflected ray will be proportional to $r^2$.

If the **Wall condition** is set to **Mixed diffuse and specular reflection**, this section is instead called **Absorption Coefficients** and the absorption coefficients for the diffusely and specularly reflected rays are specified separately. All of the text fields are given subscripts $s$ and $d$ for specularly and diffusely reflected rays, respectively.

**NEW VALUE OF AUXILIARY DEPENDENT VARIABLES**

This section is available if an Auxiliary Dependent Variable has been added to the model.

When a ray crosses or touches a boundary, the values of the user-defined auxiliary dependent variables can be changed. The value can be a function of any combinations of ray variables and variables defined on the boundary.

Select the **Assign new value to auxiliary variable** check box or boxes based on the number of auxiliary variables in the model. Then enter the new value or expression in the field. For example, if there is an auxiliary variable, psi, then enter a value for $\text{psi}_{\text{new}}$ in the field. So, to increment the value of psi by 1 when a ray touches or crosses a boundary, enter psi+1 in the text field for $\text{psi}_{\text{new}}$.

If the **Primary ray condition** is set to **Probability**, or if the **Diffuse scattering**, **Isotropic scattering**, or **Mixed diffuse and specular reflection** wall condition is used, then the **Wall** feature generates random numbers. Random numbers are also used if **Reinitialization wavelength** or **Reinitialization frequency** is activated.

If, in addition, the **Arguments for random number generation** setting is set to **User defined** in the physics interface **Advanced Settings** section, the **Advanced Settings** section is available. Enter the **Additional input argument to random number generator** $i$ (dimensionless). The default value is 1.

The **Advanced Settings** section is also shown if the **Compute optical path length** check box is selected under the physics interface **Additional Variables** section. Select the **Reset optical path length** check box to set the optical path length to 0 when a ray touches the wall.

## Mirror

Use the **Mirror** node to specularly reflect rays at a boundary. This feature functions as a special case of the **Wall** node, except that the wall condition is always specular reflection.

See Wall for information on the following sections: **Absorption Coefficient**, **Frequency Reinitialization**, **Wavelength Reinitialization**, **New Value of Auxiliary Dependent Variables**, and **Advanced Settings**.

## Ideal Lens

Use the **Ideal Lens** boundary condition to treat a surface as if it were a lens, without having to create a detailed lens geometry.

The selected boundary or boundaries for the **Ideal Lens** should generally be a planar surface (in 3D) or a straight edge (in 2D).

*Device Properties*

Select an option from the **Ideal lens type** list: **Paraxial surface** (the default), **Thin lens**, or **Thick lens**.

- If **Paraxial surface** is selected, choose one of the following from the **Paraxial surface type** list:

  - **Specify effective focal length** (the default): enter a value or expression for the **Effective focal length** $f_{eff}$ (SI unit: m). The default is 100 mm.

  - **Specify optical power**: enter a value or expression for the **Optical power** $K$ (SI unit: 1/m). The default is 0.1 m$^{-1}$.

- If **Thin lens** is selected, enter the following:

  - **Radius of curvature, surface 1** $R_1$ (SI unit: m). The default is 100 mm. This value should be positive for a convex surface or negative for a concave surface.

  - **Radius of curvature, surface 2** $R_2$ (SI unit: m). The default is 100 mm. This value should be negative for a convex surface or positive for a concave surface.

  - **Refractive index** $n$ (dimensionless). The default is 1.5.

- If **Thick lens** is selected, enter the same parameters as for **Thin lens**, plus the additional **Center thickness** $T_c$ (SI unit: m). The default is 0.

*Ideal Lens Reference*

The ideal lens reference is the pole of the ideal lens. A rays passing through this point will be undeviated. The **Ideal lens reference** can be selected from a number of options.

- **Centroid of selection** will compute the geometric center of all selected boundaries.

- **From coordinates** will give a point on the ideal lens that is a projection of a user defined point onto a plane containing the ideal lens surface.

- **Selected point** will use the point indicated in the **Reference Point Selection** section.

See Wall for information on the section **New Value of Auxiliary Dependent Variables.**

| | |
|---|---|
| ℚ | Ideal Lens Theory |

*Axial Symmetry*

The **Axial Symmetry** node is automatically added to 2D axisymmetric models. The options available for the feature are the same as for Wall, except as follows.

The **Boundary Selection** is locked and is only applicable to edges on the symmetry axis. The only wall conditions available are **Specular reflection** (the default), **Freeze**, **Stick**, and **Disappear**. In addition, the **Primary Ray Condition** section is not included. The **Axial Symmetry** boundary condition does not affect ray intensity or polarization, except to introduce a phase delay of $\pi$ in reflected rays to compensate for the change in the principal curvature direction.

---

The **Axial Symmetry** condition only applies to straight boundaries that are both on the axis of symmetry and adjacent to a domain in the selection of the physics interface. If rays are propagating in the void region outside of the selected domains, it is possible for the rays to enter the region where $r < 0$, even though no geometry is defined there.

To ensure that rays cannot propagate into the region where $r < 0$, draw line segments on the parts of the symmetry axis where no geometric entities exist, then add the **Wall** node to these edges. Keep in mind that rays can only be subjected to boundary conditions if the corresponding boundaries are meshed.

---

## *Release*

Use the **Release** node to release rays within domains based on arbitrary expressions or based on the positions of the mesh elements.

### RELEASE TIMES

This section is only available when the **Allow multiple release times** check box has been selected in the physics interface **Advanced Settings** section. Enter **Release times** (SI unit: s) or click the **Range** button ( ) to select and define a range of specific times. At each release time, rays are released with initial position and ray direction vector as defined next.

### INITIAL POSITION

Select an **Initial position**: **Density** (the default) or **Mesh based**.

*Density*

For **Density** enter a value for the **Number of rays per release** $N$ (dimensionless). The default is 100. Then enter a value or expression for the **Density proportional to** $\rho$ (dimensionless). The default is 1.

The **Density proportional to** ρ can be an expression rather than a number; the resulting ray distribution approximately has a number density that is proportional to this expression. The resulting distribution looks a bit random, and it depends on the order in which the mesh elements are numbered. The distribution is probably not exactly the same in different COMSOL Multiphysics versions, but the total number of rays released is always $N$.

| ! | The **Density proportional to** expression must be strictly positive. |
|---|---|

*Advanced Options for Density-Based Release*
The following options can be adjusted to make the number density of rays more closely conform to the **Density proportional to** expression.

Select a **Release distribution accuracy order** between **1** and **5** (the default is **5**), which determines the integration order that is used when computing the number of rays to release within each mesh element. The higher the accuracy order, the more accurately rays will be distributed among the mesh elements.

The **Position refinement factor** (default **0**) must be a nonnegative integer. When the refinement factor is **0**, each ray is always assigned a unique position, but the density is taken as a uniform value over each mesh element. If the refinement factor is a positive integer, the distribution of rays within each mesh element is weighted according to the density, but it is possible for some rays to occupy the same initial position. Further increasing the **Position refinement factor** increases the number of evaluation points within each mesh element to reduce the probability of multiple rays occupying the same initial position.

*Mesh Based*
For **Mesh based** the rays are released from a set of positions determined by a selection of geometric entities (of arbitrary dimension) in the mesh. Given a **Refinement factor** between 1 and 5, the centers of the refined mesh elements are used. Thus, the number of positions per mesh element is `refine^dim`, except for pyramids, where it is `(4*refine`$^2$`-1)*refine/3`.

**RAY DIRECTION VECTOR**

Select an option from the **Ray direction vector** list: **Expression** (the default), **Spherical**, **Hemispherical**, **Conical**, or **Lambertian** (3D only).

- For **Expression** a single ray is released in the specified direction. Enter coordinates for the **Ray direction vector** $\mathbf{L}_0$ (dimensionless) based on space dimension.

- For **Spherical** a number of rays are released at each point, sampled from a spherical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50.

- For **Hemispherical** a number of rays are released at each point, sampled from a hemispherical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then enter coordinates for the **Hemisphere axis** $\mathbf{r}$ based on space dimension.

- For **Conical** a number of rays are released at each point, sampled from a conical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then enter coordinates for the **Cone axis** $\mathbf{r}$ based on space dimension. Then enter the **Cone angle** $a$ (SI unit: rad). The default value is $\pi/3$ radians.

- The **Lambertian** option is only available in 3D. A number of rays are released at each point, sampled from a hemisphere in wave vector space with probability density based on the cosine law. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then enter coordinates for the **Hemisphere axis** $\mathbf{r}$ based on space dimension.

If **Conical** is selected in a 3D model, select an option from the **Conical distribution** list:

- **Uniform density** (the default): rays are released with polar angles from 0 to the specified cone angle. The rays are distributed in wave vector space so that each ray subtends approximately the same solid angle.

- **Specify polar and azimuthal distributions**: specify the **Number of polar angles** $N_\theta$ (dimensionless) and the **Number of azimuthal** angles $N_\varphi$ (dimensionless). Rays are released at uniformly distributed polar angles from 0 to the specified cone angle. A single axial ray ($\theta = 0$) is also released. For each value of the polar angle, rays are released at uniformly distributed azimuthal angles from 0 to $2\pi$. Unlike other options for specifying the conical distribution, it is not necessary to directly specify the **Number of rays in wave vector space** $N_w$ (dimensionless), which is instead derived from the relation $N_w = N_\theta \times N_\varphi + 1$.

- **Hexapolar**: specify the **Number of polar angles** $N_\theta$ (dimensionless). In this distribution, for each release point, one ray will be released along the cone axis. Six

rays are released at an angle $\alpha/N_\theta$ from the cone axis, then 12 additional rays at an angle of $2\alpha/N_\theta$, and so on. The total number of ray directions in the distribution is $N_w = 3N_\theta(N_\theta + 1) + 1$.

- **Flat**: rays are released in a flat fan shape within the specified angle.

- **Marginal rays only:** the rays are all released at an angle $\alpha$ with respect to the cone axis. The rays are released at uniformly distributed azimuthal angles from 0 to $2\pi$.

- **Marginal and axial rays only:** the rays are all released at an angle $\alpha$ with respect to the cone axis, except for one ray which is released along the cone axis. The marginal rays are released at uniformly distributed azimuthal angles from 0 to $2\pi$.



*Figure 3-3: Comparison of the available cone-based release distributions.*

In 3D for the **Conical distribution** you can also let the **Transverse direction** be **Automatic** (the default) or **User defined**. For **User defined** enter the components of $\mathbf{e}_t$. This controls, for example, the orientation of the ray fan when **Flat** is selected.

For **Spherical**, **Hemispherical**, **Conical**, and **Lambertian**, select an option from the **Sampling from Distribution** list: **Deterministic** (the default) or **Random**. If **Deterministic** is selected, the initial ray direction vectors are computed using an algorithm that seeks to distribute the rays as evenly as possible in wave vector space. This algorithm will give the same initial ray directions whenever the study is run. If **Random** is selected, the initial direction of each ray is sampled from a probability distribution in wave vector space using pseudorandom numbers. The result may be the same when rerunning the study multiple times on the same computer, but the solution is likely to be different on different architectures.

This section is available when **Polychromatic, specify frequency** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section.

Select a **Distribution function**: **None** (the default), **Normal**, **Lognormal**, **Uniform**, **Blackbody**, or **List of values**.

When **None** is selected, enter an initial value $\nu_0$ (SI unit: Hz). The default value is $4.54 \times 10^{14}$ Hz.

Select **Normal** to create a normal distribution function, **Lognormal** to create a log-normal distribution function, **Uniform** to create a uniform distribution function, or **Blackbody** to sample values according to Planck's law for blackbody radiation. For any of these distributions, select an option from the **Sampling from distribution** check box: **Deterministic** (the default) or **Random**. For **Random** sampling the mean and standard deviation may not be exactly equal to the expected values but will statistically converge as the number of rays is increased. The **Number of values** sets the number of values that are sampled from the distribution function at each release point.

For the **Normal** or **Lognormal** distribution enter a user-defined **Mean ray frequency** (default $4.54 \times 10^{14}$ Hz) and **Ray frequency standard deviation** (default $10^{14}$ Hz). For the **Uniform** distribution enter the **Minimum ray frequency** $\nu_{min}$ (default $4.3 \times 10^{14}$ Hz) and **Maximum ray frequency** $\nu_{max}$ (default $7.5 \times 10^{14}$ Hz). Select **List of values** to enter a list of distinct frequency values.

For **Blackbody**, enter the **Blackbody temperature** $T_{bb}$ (SI unit: K). The default value of 5780 K is an approximate value for treating the sun as a blackbody radiation source. Then select an option from the **Distribution type** list: **Specify fraction of total emissive power** (the default), or **Specify bandwidth**.

- If **Specify fraction of total emissive power** is selected, enter the **Fraction of total emissive power** $f_{bb}$ (dimensionless). The default is 0.95.

- If **Specify bandwidth** is selected, enter the **Minimum ray frequency** $\nu_{min}$ and **Maximum ray frequency** $\nu_{max}$ (SI unit: Hz). The defaults are $4.3 \times 10^{14}$ Hz and $7.5 \times 10^{14}$ Hz, respectively.

VACUUM WAVELENGTH

This section is available when **Polychromatic, specify vacuum wavelength** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section.

Select a **Distribution function**: **None** (the default), **Normal**, **Lognormal**, **Blackbody**, **Uniform**, or **List of values**.

When **None** is selected, enter a value or expression for the **Vacuum wavelength** $\lambda_0$ (SI unit: m). The default is 660 nm. All rays released by this feature will have the same wavelength.

Select **Normal** to create a normal distribution function, **Lognormal** to create a log-normal distribution function, **Uniform** to create a uniform distribution function, or **Blackbody** to sample values according to Planck's law for blackbody radiation. For any of these distributions, select an option from the **Sampling from distribution** check box: **Deterministic** (the default) or **Random**. For **Random** sampling the mean and standard deviation may not be exactly equal to the expected values but will statistically converge as the number of rays is increased. The **Number of values** sets the number of values that are sampled from the distribution function at each release point.

For the **Normal** or **Lognormal** distribution enter a user-defined **Mean vacuum wavelength** (default 660 nm) and **Vacuum wavelength standard deviation** (default 100 nm). For the **Uniform** distribution enter the **Minimum vacuum wavelength** $\lambda_{0,\mathrm{min}}$ (default 400 nm) and **Maximum vacuum wavelength** $\lambda_{0,\mathrm{max}}$ (default 700 nm). Select **List of values** to enter a list of distinct wavelength values directly.

For **Blackbody**, enter the **Blackbody temperature** $T_{\mathrm{bb}}$ (SI unit: K). The default value of 5780 K is an approximate value for treating the sun as a blackbody radiation source. Then select an option from the **Distribution type** list: **Specify fraction of total emissive power** (the default), or **Specify bandwidth**.

- If **Specify fraction of total emissive power** is selected, enter the **Fraction of total emissive power** $f_{\mathrm{bb}}$ (dimensionless). The default is 0.95.

- If **Specify bandwidth** is selected, enter the **Minimum vacuum wavelength** $\lambda_{0,\mathrm{min}}$ and **Maximum vacuum wavelength** $\lambda_{0,\mathrm{max}}$ (SI unit: m). The defaults are 400 nm and 700 nm, respectively.

### INITIAL PHASE

This section is available when the **Compute phase** check box is selected under the physics interface **Intensity Computation** section. Enter an **Initial phase** $\Psi_0$ (SI unit: rad). The default value is 0.

### INITIAL INTENSITY

This section is available when the ray intensity is solved for in the model and **Expression** is selected as the **Ray direction vector**. Enter a value for the **Initial intensity** $I_0$ (SI unit: $W/m^2$). The default is $1000 \, W/m^2$.

### INITIAL RADII OF CURVATURE

This section is available when the ray intensity is solved for in the model and **Expression** is selected as the **Ray direction vector**. Select a **Wavefront shape**. In 3D the available options are **Plane wave** (the default), **Spherical wave**, and **Ellipsoid**. In 2D the available options are **Plane wave** (the default) and **Cylindrical wave**.

- For an idealized plane wave the radii of curvature would be infinite. However, because the algorithm used to compute intensity requires finite values, when **Plane wave** is selected the initial radii of curvature are instead given an initial value that is $10^8$ times greater than the characteristic size of the geometry.

- For a **Spherical wave** or **Cylindrical wave**, enter the **Initial radius of curvature** $r_0$ (SI unit: m).

- For an **Ellipsoid**, enter the **Initial radius of curvature, 1** $r_{1,0}$ (SI unit: m) and the **Initial radius of curvature, 2** $r_{2,0}$ (SI unit: m). Also enter the **Initial principal curvature direction, 1** $e_{1,0}$ (dimensionless).

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⚠️  For spherical and cylindrical waves the **Initial radius of curvature** must be nonzero. To release a ray such that the initial wavefront radius of curvature is zero, instead select a different option such as **Conical** from the **Ray direction vector** list.

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🔍  Principal Radii of Curvature

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### INITIAL POLARIZATION

This section is available when the ray intensity or power is solved for.

Select an **Initial polarization type**: **Unpolarized** (the default), **Fully polarized**, or **Partially polarized**.

Select an **Initial polarization**: **Along principal curvature direction** (the default) or **User defined**.

- For **Fully polarized** and **Partially polarized** rays in 3D enter an **Initial polarization parallel to reference direction** $a_{1,0}$ (dimensionless), **Initial polarization perpendicular to reference direction** $a_{2,0}$ (dimensionless), and **Initial phase difference** $\delta_0$ (SI unit: rad).

- For **Fully polarized** and **Partially polarized** rays in 2D enter an **Initial polarization, in plane** $a_{xy,1}$ (dimensionless), **Initial polarization, out of plane** $a_{z,0}$ (dimensionless), and **Initial phase difference** $\delta_0$ (SI unit: rad).

- For **User defined** also enter an **Initial polarization reference direction** $\mathbf{u}$ (dimensionless).

For **Partially polarized**, also enter an **Initial degree of polarization** $P_0$ (dimensionless).

**TOTAL SOURCE POWER**

This section is available:

- when the ray intensity is solved for, and

- when **Spherical**, **Hemispherical**, or **Conical** is selected as the **Ray direction vector**.

- It is also available when the ray power is solved for, and then any choice of **Ray direction vector** displays this section.

Select an option from the **Intensity initialization** list: **Uniform distribution** (the default) or **Weighted distribution**. If any Photometric Data Import nodes have been added to the model then they can also be selected from the list.

If **Uniform distribution** or **Weighted distribution** is selected, enter a **Total source power** $P_{\mathrm{src}}$ (SI unit: W). The default is 1 W. In 2D, instead enter the **Total source power per unit thickness** $P_{\mathrm{src}}$ (SI unit: W/m). The default is 1 W/m. For **Weighted distribution**, also enter an expression for the **Power weighting factor** $P_{\mathrm{wt}}$. The weighting factor may have any unit; the default expression is 1. The released rays will have initial intensity

and power proportional to the weighting factor, while still adding up to the specified source power.

| | For example, if you release 1000 rays in a **Spherical** distribution with an initial power of 10 W, and enter a weighting factor of gop.niz+1, then the sum of the power over all released rays, gop.sum(gop.Q), will equal 10 W. Since gop.niz is the $z$-component of the ray direction vector, rays close to the $z$-axis will each have power of about 0.02 W, those around the negative $z$ direction will have almost no power, and those in the $xy$-plane will each have power of about 0.01 W. |
|---|---|

If any **Photometric Data Import** feature is selected from the list, the source power is instead obtained directly from the imported photometric data (IES) file. Enter values or expressions for the components of the **Photometric horizontal** $\mathbf{p}_h$ (dimensionless) and **Photometric zero** $\mathbf{p}_z$ (dimensionless). By default, these vectors point in the directions of the positive $x$- and $z$-axes, respectively.

| | The relationship between the photometric horizontal, photometric vertical, and ray direction vector, and its effect on the initial ray intensity, is explained in ANSI/IESNA LM-63-02 (R2008), *IESNA Standard file format for the electronic transfer of photometric data and related information*, Illuminating Engineering Society (2002). |
|---|---|

| ⚠ | The **Photometric Data Import** feature does not support the options TILT=INCLUDE or TILT=<FILENAME> that are included in some IES files. Only TILT=NONE is allowed. |
|---|---|

### INITIAL VALUE OF AUXILIARY DEPENDENT VARIABLES

For each of the Auxiliary Dependent Variable nodes added to the model, select a **Distribution function** for the initial value of the auxiliary dependent variables and whether the initial value of the auxiliary dependent variables should be a scalar value or sampled from a distribution function.

The number of rays simulated can increase substantially and the following options are available for each **Auxiliary Dependent Variable** added to the model.

When **None** is selected, enter an initial value. The symbol for the initial value is the auxiliary variable name followed by a subscript 0, so for the default name rp the initial value has symbol $rp_0$.

For the initial value of the auxiliary dependent variables, select **Normal** to create a normal distribution function, **Lognormal** to create a log-normal distribution function, or **Uniform** to create a uniform distribution function. For any of these distributions, select an option from the **Sampling from distribution** check box: **Deterministic** (the default) or **Random**. For **Random** sampling the mean and standard deviation may not be exactly equal to the specified values but will statistically converge as the number of rays is increased. The **Number of values** sets the number of values that are sampled from the distribution function at each release point.

For the **Normal** or **Lognormal** distribution enter the **Mean** (default 0) and **Standard deviation** (default 1). For the **Uniform** distribution enter the **Minimum** (default 0) and **Maximum** (default 1). Select **List of values** to enter a set of numerical values directly.

By default auxiliary dependent variables are initialized after all other degrees of freedom. Select the **Initialize before wave vector** check box to compute the initial value of the auxiliary dependent variable immediately after computing the initial wave vectors of the rays. By selecting this check box it is possible to define the initial ray direction as a function of the auxiliary dependent variables.

## *Release from Boundary*

Use the **Release from Boundary** node to determine how to release rays on an interior or exterior boundary in a specific direction.

The Nonlocal Accumulator subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

See Release for information on the following sections: **Release Times**, **Initial Ray Frequency**, **Vacuum Wavelength**, **Initial Phase**, **Initial Intensity**, **Total Source Power**, **Initial Polarization**, and **Initial Value of Auxiliary Dependent Variables**.

### COORDINATE SYSTEM SELECTION

It is possible to specify the initial ray direction in terms of the global coordinates or in another coordinate system defined for the model Component. Select an option from the **Coordinate system** list. By default **Global coordinate system** is selected. If other coordinate systems are defined, they can also be selected from the list. When specifying the initial ray direction (see the **Ray Direction Vector** section), direction components can

be specified using the basis vectors of whichever coordinate system has been selected from the list.

When a coordinate system other than **Global coordinate system** is selected from the **Coordinate system** list, arrows will appear in the Graphics window to indicate the orientation of the basis vectors of the coordinate system on the selected boundaries.

### INITIAL POSITION

Select an **Initial position**: **Uniform distribution** (the default for 2D components) **Projected plane grid** (the default for 3D components), **Mesh based**, or **Density**. Mesh based and Density have the same settings as described for the Release node.

|   |   |
|---|---|
| Ω | For 2D components, if **Uniform distribution** is selected, enter the **Number of rays per release** $N$ (dimensionless). The union of the selected boundaries is divided into $N$ segments of approximately equal length, and a ray is placed in the middle of each segment. |

|   |   |
|---|---|
|  | For 3D components, if **Projected plane grid** is selected, enter the **Number of rays per release** $N$ (dimensionless). The rays are distributed on a plane grid in planes that are approximately tangential to the selected boundaries (for a plane boundary, you get a uniform distribution). |

### RAY DIRECTION VECTOR

Select an option from the **Ray direction vector** list: **Expression** (the default), **Hemispherical**, **Conical**, or **Lambertian** (3D only).

- For **Expression** a single ray is released in the specified direction. Enter coordinates for the **Ray direction vector** $\mathbf{L}_0$ (dimensionless) based on space dimension. Select the **Specify tangential and normal vector components** check box to specify the initial direction using a coordinate system based on the directions tangential and normal to the surface $(t_1, t_2, n)$.

- For **Hemispherical** a number of rays are released at each point, sampled from a hemispherical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_\mathrm{w}$ (dimensionless). The default is 50. Then enter coordinates for the **Hemisphere axis r** based on space dimension. Select the **Specify tangential and normal vector components** check box to specify the hemisphere axis using a coordinate system based on the directions tangential and normal to the surface $(t_1, t_2, n)$.

- For **Conical** a number of rays are released at each point, sampled from a conical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then enter coordinates for the **Cone axis r** based on space dimension. Then enter the **Cone angle** $\alpha$ (SI unit: rad). The default value is $\pi/3$ radians. Select the **Specify tangential and normal vector components** check box to specify the cone axis using a coordinate system based on the directions tangential and normal to the surface $(t_1, t_2, n)$.

- The **Lambertian** option is only available in 3D. A number of rays are released at each point, sampled from a hemisphere in wave vector space with probability density based on the cosine law. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then enter coordinates for the **Hemisphere axis r** based on space dimension. Select the **Specify tangential and normal vector components** check box to specify the hemisphere axis using a coordinate system based on the directions tangential and normal to the surface $(t_1, t_2, n)$.

---

When the **Specify tangential and normal vector components** check box is selected, arrows indicating the normal direction on the selected boundaries will appear in the Graphics window.

Note that the normal direction may be opposite the built-in variable for the boundary normal (for example, nx, ny, and nz) to ensure that a positive value causes rays to be released into the simulation domain. This often occurs when the release is applied to exterior boundaries.

When the normal direction used by the **Release from Boundary** feature is opposite the normal vector defined by the geometry, the tangential directions are similarly inverted to ensure that the boundary coordinate system is right-handed.

---

If **Conical** is selected in a 3D model, select an option from the **Conical distribution** list:

- **Uniform density** (the default): rays are released with polar angles from 0 to the specified cone angle. The rays are distributed in wave vector space so that each ray subtends approximately the same solid angle.

- **Specify polar and azimuthal distributions**: specify the **Number of polar angles** $N_\theta$ (dimensionless) and the **Number of azimuthal** angles $N_\varphi$ (dimensionless). Rays are released at uniformly distributed polar angles from 0 to the specified cone angle. A single axial ray ($\theta = 0$) is also released. For each value of the polar angle, rays are released at uniformly distributed azimuthal angles from 0 to $2\pi$. Unlike other

options for specifying the conical distribution, it is not necessary to directly specify the **Number of rays in wave vector space** $N_w$ (dimensionless), which is instead derived from the relation $N_w = N_\theta \times N_\varphi + 1$.

- **Hexapolar**: specify the **Number of polar angles** $N_\theta$ (dimensionless). In this distribution, for each release point, one ray will be released along the cone axis. Six rays are released at an angle $\alpha/N_\theta$ from the cone axis, then 12 additional rays at an angle of $2\alpha/N_\theta$, and so on. The total number of ray directions in the distribution is $N_w = 3N_\theta(N_\theta + 1) + 1$.

- **Flat**: rays are released in a flat fan shape within the specified angle.

- **Marginal rays only**: the rays are all released at an angle $\alpha$ with respect to the cone axis. The rays are released at uniformly distributed azimuthal angles from 0 to $2\pi$.

- **Marginal and axial rays only**: the rays are all released at an angle $\alpha$ with respect to the cone axis, except for one ray which is released along the cone axis. The marginal rays are released at uniformly distributed azimuthal angles from 0 to $2\pi$.

The available **Conical distribution** options are illustrated in Figure 3-3.

In 3D for the **Conical distribution** you can also let the **Transverse direction** be **Automatic** (the default) or **User defined**. For **User defined** enter the components of $\mathbf{e}_t$. This controls, for example, the orientation of the ray fan when **Flat** is selected.

For **Hemispherical**, **Conical**, and **Lambertian**, select an option from the **Sampling from Distribution** list: **Deterministic** (the default) or **Random**. If **Deterministic** is selected, the initial ray direction vectors are computed using the same algorithm, which seeks to distribute the rays as evenly as possible in wave vector space, whenever the study is run. If **Random** is selected, the initial direction of each ray is sampled from a probability distribution in wave vector space using pseudorandom numbers.

### INITIAL RADII OF CURVATURE

This section is available when the ray intensity is solved for in the model and **Expression** is selected as the **Ray direction vector**. Select a **Wavefront shape**. In 3D the available

options are **From surface curvature** (the default), **Plane wave**, **Spherical wave**, and **Ellipsoid**. In 2D the available options are **Plane wave** (the default) and **Cylindrical wave**.

- For a **Spherical wave** or **Cylindrical wave**, enter the **Initial radius of curvature** $r_0$ (SI unit: m).

- For an **Ellipsoid** (3D only), enter the **Initial radius of curvature, 1** $r_{1,0}$ (SI unit: m) and the **Initial radius of curvature, 2** $r_{2,0}$ (SI unit: m). Also enter the **Initial principal curvature direction, 1** $\mathbf{e}_{1,0}$ (dimensionless).

> ⚠️ For spherical and cylindrical waves the **Initial radius of curvature** must be nonzero. To release a ray such that the initial wavefront radius of curvature is zero, instead select a different option such as **Conical** from the **Ray direction vector** list.

> 🔍 Principal Radii of Curvature

*Release from Symmetry Axis*

Use the **Release from Symmetry Axis** node to release rays from specified edges along the axis of symmetry in a 2D axisymmetric geometry. It functions like the Release from Boundary node, except that it can only be applied to the axis of symmetry and that the options in the **Ray Direction Vector** section are slightly different.

See Release for information on the following sections: **Release Times, Initial Ray Frequency**, **Vacuum Wavelength**, **Initial Phase**, **Initial Intensity**, **Initial Radii of Curvature**, **Total Source Power**, **Initial Polarization**, and **Initial Value of Auxiliary Dependent Variables**.

**INITIAL POSITION**

Select an **Initial position**: **Uniform distribution** (the default), **Mesh based**, or **Density**. **Mesh based** and **Density** have the same settings as described for the Release node.

If **Uniform distribution** is selected, enter the **Number of rays per release** $N$ (dimensionless). The default is 100. The set of the selected boundaries is divided into $N$ segments of approximately equal length, with one ray at the middle of each segment.

## RAY DIRECTION VECTOR

Select an option from the **Ray direction vector** list: **Expression** (the default), **Spherical**, or **Conical**.

- For **Expression** a single ray is released in the specified direction. Enter the radial and axial components of the **Ray direction vector** $\mathbf{L}_0$ (dimensionless).

- For **Spherical** a number of rays are released at each point, from the negative $z$ direction to the positive $z$ direction in the half plane with $r > 0$. These rays are sampled from an anisotropic hemispherical distribution in wave vector space, so that rays are more heavily weighted toward the $r$ direction rather than the $\pm z$ directions. In 3D this would correspond to a spherical distribution of rays such that each ray subtends approximately the same solid angle in wave vector space.

  Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then enter coordinates for the **Hemisphere axis r** based on space dimension. Select the **Specify tangential and normal vector components** check box to specify the hemisphere axis using a coordinate system based on the directions tangential and normal to the surface $(t_1, t_2, n)$.

- For **Conical** a number of rays are released at each point, sampled from a conical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then enter coordinates for the **Cone axis r** based on space dimension. Then enter the **Cone angle** $\alpha$ (SI unit: rad). The default value is $\pi/3$ radians. Unlike the **Spherical** distribution, the rays in the **Conical** distribution each subtend the same angle in 2D, not the same solid angle in 3D.

For **Hemispherical** and **Conical**, select an option from the **Sampling from Distribution** list: **Deterministic** (the default) or **Random**. If **Deterministic** is selected, the initial ray direction vectors are computed using the same algorithm, which seeks to distribute the rays as evenly as possible in wave vector space, whenever the study is run. If **Random** is selected, the initial direction of each ray is sampled from a probability distribution in wave vector space using pseudorandom numbers.

## *Release from Edge*

Use the **Release from Edge** node to release rays from positions along a set of edges in a 3D geometry.

The **Initial Position** section is described below. For all other sections, see Release.

Select an **Initial position**: **Mesh based** (the default), **Uniform distribution**, or **Density**. Mesh based and Density have the same settings as described for the Release node. If **Uniform distribution** is selected, enter the **Number of rays per release** $N$ (dimensionless). The union of the selected edges is divided into $N$ segments of approximately equal length, and a ray is released from the middle of each segment.

## Release from Point

Use the **Release from Point** node to release rays from a set of points in a geometry. By default one ray is released at every selected point, although it is possible to release multiple rays at each point if the initial direction or an auxiliary dependent variable is sampled from a distribution.

For information on the settings, see Release.

## Release from Point on Axis

The **Release from Point on Axis** feature is similar to the Release from Point feature, except that the points must be on the axis of symmetry in a 2D axisymmetric geometry.

See Release from Boundary for information on the **Ray Direction Vector** section.

For all other sections, see Release from Point.

## Release from Grid

Use the **Release from Grid** node to release rays from a user-defined grid of points.

The **Initial Coordinates** section is described below. For all other sections, see Release.

INITIAL COORDINATES

Select an option from the **Grid type** list: **All combinations** (the default), **Specified combinations**, **Cylindrical** (3D only), or **Hexapolar** (3D only).

*Linear, Rectangular, and Arbitrary Grids*
For **All combinations** and **Specified combinations** enter **Initial coordinates** based on space dimension ($q_{x,0}$, $q_{y,0}$, and $q_{z,0}$ for 3D components) for the ray positions or click the **Range** button ( ⌊⌟ ) to select and define a range of specific coordinates.

If **Specified combinations** is selected, the number of initial coordinates entered for each space dimension must be equal, and the total number of rays released is equal to the

length of one of the lists of initial coordinates. If **All combinations** is selected, the total number of rays released is equal to the product of the lengths of each list of initial coordinates.

For example, suppose a 2D component includes a **Release from Grid** node with the following initial coordinates:

- $q_{x,0}$ = range(0,1,3)
- $q_{y,0}$ = range(2,2,8)

If **All combinations** is selected, a total of **16** rays will be released, including every possible combination of the initial $x$- and $y$-coordinates. If **Specified combinations** is selected, 4 rays will be released with initial positions (0,2), (1,4), (2,6), and (3,8).

*Cylindrical Grids*

For **Cylindrical**, enter coordinates for the **Center location** $\mathbf{q}_c$ (SI unit: m). By default, the distribution is centered at the origin. Then enter the components of the **Cylinder axis direction** $\mathbf{r}_c$ (dimensionless). The rays will be released at specified radial distances and angles in the plane containing the point $\mathbf{q}_c$ and orthogonal to the direction $\mathbf{r}_c$.

Select an option from the **Radial distribution** list: **Uniform radius intervals** (the default), **Uniform number density**, or **User defined**.

For **Uniform radius intervals** or **Uniform number density** enter a value or expression for the **Radius** $R_c$ (SI unit: m). The default is **1** m. Then enter a positive integer for the **Number of radial positions** $N_c$ (dimensionless). The default is **5**.

For **User defined** enter a list of **Radial coordinates** $q_r$ (SI unit: m) directly. An arbitrary number of radial coordinates can be entered in the list. The default is **1** m.

The effect of the **Radial distribution** setting on the resulting ray placement is illustrated in Figure 3-4. For **Uniform radius intervals**, the distances between the concentric rings of rays are all equal, but the number density of rays is greater at the center of the distribution than at the outer edge. The option **Uniform number density** corrects this imbalance by defining nonuniform increments in the radial position between the concentric rings.

Enter a positive integer for the **Number of angles** $N_\varphi$ (dimensionless). The default is **10**.

The total number of rays released (before accounting for distributions of ray direction or auxiliary dependent variables at each release point) is $N_c \times N_\phi + 1$ because a single ray is also released at the center of the distribution.
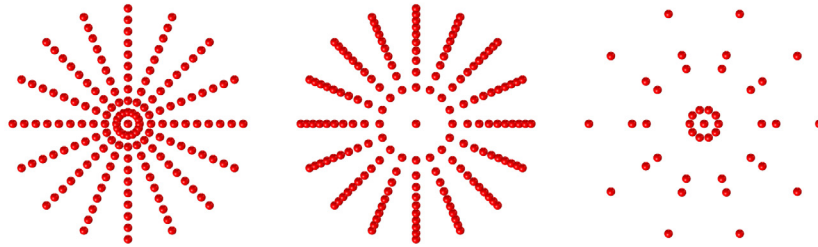


*Figure 3-4: Comparison of the cylindrical release in which rays are positioned at uniform radius intervals (left), with uniform number density (center), or at user-defined radii (right).*

### Hexapolar Grids

For **Hexapolar**, enter coordinates for the **Center location $\mathbf{q}_c$** (SI unit: m). By default, the distribution is centered at the origin. Then enter the components of the **Cylinder axis direction $\mathbf{r}_c$** (dimensionless). The rays will be released at specified radial distances and angles in the plane containing the point $\mathbf{q}_c$ and orthogonal to the direction $\mathbf{r}_c$.

Enter a value or expression for the **Radius $R_c$** (SI unit: m). The default is 1 m. Then enter a positive integer for the **Number of radial positions $N_c$** (dimensionless). The default is 5.

Unlike the **Cylindrical** grid types described in the previous section, each concentric ring of the **Hexapolar** grid releases a different number of rays, as shown in Figure 3-5. One ray is always released at the center. The first ring of rays surrounding the center has 6 rays arranged in a regular hexagon. Each ring of rays beyond the first has 6 more rays than the ring preceding it, with the grid points arranged in a regular polygon. The radius increments between consecutive rings are uniform.

The total number of grid points generated is

$$N_{\text{grid}} = 1 + 3N_c(N_c + 1)$$

Thus the relationship between the number of radius intervals and the total number of grid points is quadratic.
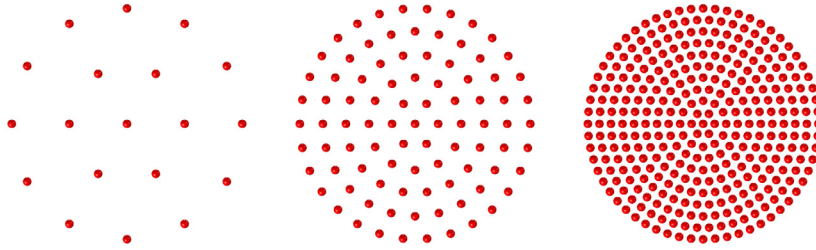


*Figure 3-5: Comparison of hexapolar grids with 2 rings (left), 5 (middle), and 10 (right).*

*Previewing Grid Points*

In the **Initial Coordinates** section, you can click the **Preview Initial Coordinates** and **Preview Initial Extents** buttons to visualize the ray release positions. Clicking **Preview Initial Coordinates** will cause a point to appear in the Graphics window for every release position. Clicking **Preview Initial Extents** will cause a bounding box to appear, indicating the spatial extents of the released rays. Examples are shown in Figure 3-6 and Figure 3-7.
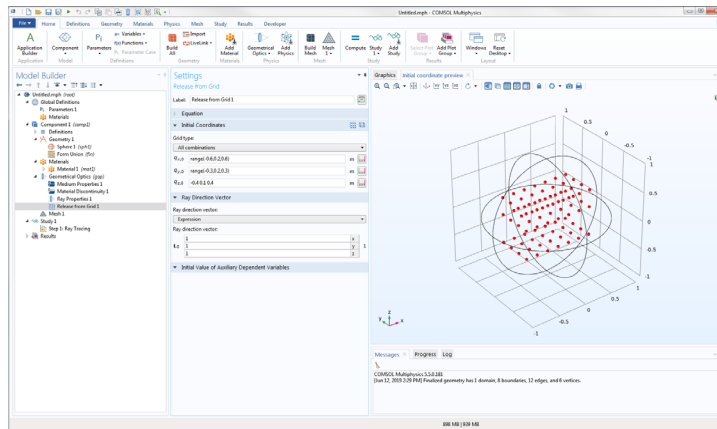


*Figure 3-6: Graphics window after clicking the Preview Initial Coordinates button.*
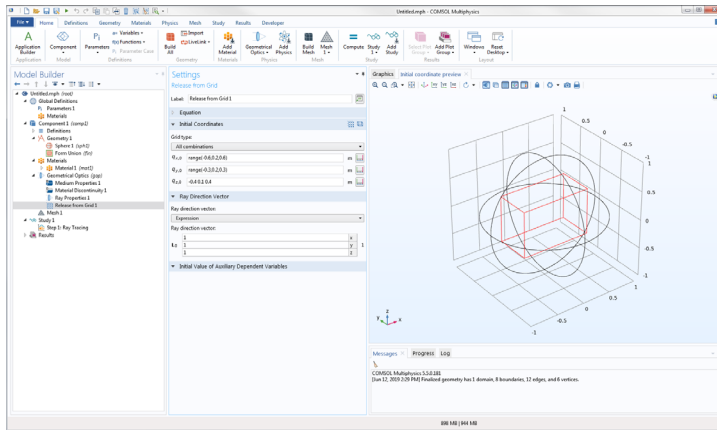
*Figure 3-7: Graphics window after clicking the Preview Initial Extents button.*

## Release from Grid on Axis

The **Release from Grid on Axis** feature is similar to the Release from Grid feature, except that it can only release rays from a grid of points along the axis of symmetry in a 2D axisymmetric geometry; that is, $q_{r,0} = 0$ for all released rays.

See Release from Boundary for information on the **Ray Direction Vector** section.

For all other sections, see Release from Grid.

## Release from Data File

Use a **Release from Data File** node to specify the initial ray position, direction, and values of auxiliary dependent variables using data from a text file.

See Release for information on the following sections: **Release Times, Initial Phase**, **Initial Intensity**, **Initial Radii of Curvature**, **Total Source Power**, and **Initial Polarization**.

### Formatting Guidelines for Files Containing Ray Data

The imported data file should be a text file (`*.txt`) arranged in a spreadsheet format; that is, each row corresponds to a distinct ray and should have the same number of columns as all other rows. Columns can be separated by spaces, tabs, or a combination of the two. Begin a line with the percent ("`%`") character to include comments or empty lines in the data file.

For example, a data file containing the following text would release rays at the positions (0.1, 0.2, 0.6) and (0.2, 0.4, 0.8) in a three-dimensional geometry:

```
% Ray release positions
% qx0 qy0 qz0
0.1 0.2 0.6
0.2 0.4 0.8
```

### INITIAL POSITION

**Browse** your computer to select a text file, then click **Import** to import the data. To remove the imported data, click **Discard**. Enter the **Index of first column containing position data** $i$ to indicate which column represents the first coordinate of the ray position vectors. The default value, 0, indicates the first column.

### TRANSFORMATIONS

The distribution of loaded ray release positions may be scaled, rotated, and translated before the rays are released.

To scale the distribution of release positions, enter a value or expression for the **Scale factor** $R$ (dimensionless). The default is 1. This scale factor can be used to correct unit discrepancies between the data file and the model geometry. For example, if the geometry length unit is in meters but the data file lists coordinates in millimeters, enter a scale factor of 0.001.

To rotate the distribution, enter the **Euler angles (Z-X-Z)** $\alpha$, $\beta$, and $\gamma$ (in 3D) or the **Rotation angle** $\alpha$ (in 2D). The default values are all 0.

In 3D, $\alpha$ is the rotation angle about the space-fixed $z$-axis, then $\beta$ is the rotation angle about the transformed $x$-axis (or $x'$-axis), and finally $\gamma$ is the rotation angle about the transformed $z$-axis (or $z''$-axis). Positive values indicate counterclockwise rotations.

Enter values or expressions for the components of the **Displacement** vector $\Delta\mathbf{q}$ (SI unit: m). The default is not to apply any translation.

If a translation and another type of transformation (scaling or rotation) are applied, then the translation is always applied after the other transformations.

### RAY DIRECTION VECTOR

Select an option from the **Ray direction vector** list: **Expression** (the default), **From file**, **Spherical**, **Hemispherical**, **Conical**, or **Lambertian** (3D only).

- For **From file**, enter the **Index of first column containing direction data** $i$. The default is 3. The columns are zero-indexed; that is, an index of 0 corresponds to the first

column. If you chose to rotate the loaded ray release positions in the **Initial Position** section, select the **Rotate initial directions** check box to apply the same rotation to the initial direction of the released rays. The check box is cleared by default.

• For all other settings, the settings are the same as for the Release node.

### INITIAL RAY FREQUENCY

This section is available when **Polychromatic, specify frequency** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section.

Select a **Distribution function**: **None** (the default), **Normal**, **Lognormal**, **Uniform**, **List of values**, or **From file**.

• When **From file** is selected, enter the **Index of column containing frequency data**. The default value is 3. The columns are zero-indexed; that is, an index of 0 corresponds to the first column.

• For all other options, the settings are the same as for the Release node.

### VACUUM WAVELENGTH

This section is available when **Polychromatic, specify vacuum wavelength** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section.

Select a **Distribution function**: **None** (the default), **Normal**, **Lognormal**, **Uniform**, **List of values**, or **From file**.

• When **From file** is selected, enter the **Index of column containing wavelength data**. The default value is 3. The columns are zero-indexed; that is, an index of 0 corresponds to the first column.

• For all other options, the settings are the same as for the Release node.

### INITIAL VALUE OF AUXILIARY DEPENDENT VARIABLES

This section is available if an Auxiliary Dependent Variable has been added to the model.

For each of the active **Auxiliary Dependent Variable** nodes in the model, choose an option from the **Distribution function** list: **From file**, **None** (the default), **Normal**, **Lognormal**, **Uniform**, or **List of Values**.

- When **From file** is selected, enter the **Index of column containing data**. The default value is 3. The columns are zero-indexed; that is, an index of 0 corresponds to the first column.

For all other options, the settings are the same as for the Release node.

### *Photometric Data Import*

📝 | The **Photometric Data Import** node is only available in 3D, and only if the ray intensity is solved for in the model.

Use the **Photometric Data Import** node to import photometric data files that can be used to initialize the ray intensity and power as a function of the initial ray direction. The **Photometric Data Import** node supports the `*.ies` file extension, the standard photometric data file format of the Illuminating Engineering Society of North America (IESNA).

#### PHOTOMETRIC DATA IMPORT

Enter a **File name**, or click the **Browse** button to locate a photometric data file. When a valid file path has been entered, click the **Import** button to load the photometric data into the model. A shortened version of the name of the photometric data file will then be displayed, along with a **Discard** button. Click the **Discard** button to discard the loaded photometric data and clear the **File name** field.

#### *Photometric Data Formatting*
The format of the imported photometric data file must be consistent with ANSI/ IESNA LM-63-02 (R2008), *IESNA Standard file format for the electronic transfer*

*of photometric data and related information*, Illuminating Engineering Society (2002).

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After creating an instance of the **Photometric Data Import** feature and loading an appropriately formatted IES file into the model, initialize the ray intensity as a function of initial ray direction by changing the following settings in a ray release feature such as the Release or Release from Grid feature:

- Select **Spherical**, **Hemispherical**, **Conical**, or **Lambertian** from the **Ray direction vector** list in the physics feature **Ray Direction Vector** section.

- Locate the **Total Source Power** section. From the **Intensity initialization** list, select an instance of the **Photometric Data Import** feature.

- Enter values or expressions for the **Photometric horizontal** and **Photometric zero** directions.

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*Gaussian Beam*

Use the **Gaussian Beam** feature to release rays with a Gaussian distribution of intensity or power. Since the Geometrical Optics interface does not consider diffraction effects, the **Gaussian Beam** node can be used in two different asymptotic limits: to release a collimated beam over short distances, or to treat the beam waist as a point source and trace rays over very long distances.

This feature is only available when either the ray intensity or power is solved for; it will not be available if **None** is selected from the physics interface **Intensity computation** list.

The **Gaussian Beam** node does not require a selection because it is not necessary to release the rays at a boundary or even within a domain; the waist may be located at an arbitrary location in the geometry (2D or 3D) or an arbitrary location along the *z*-axis (2D axisymmetric).

See Release for information on the following sections: **Release Times**, **Initial Phase**, and **Initial Value of Auxiliary Dependent Variables**.

**BEAM POSITION AND DIRECTION**

Enter the **Beam waist position** $\mathbf{q}_w$ (SI unit: m) based on space dimension. By default the beam waist is located at the origin. Then enter the **Beam axis r** (dimensionless)

based on space dimension. By default this is the positive $z$ direction in 3D or the positive $x$ direction in 2D.

In a 2D axisymmetric geometry, the position and orientation of the Gaussian beam is more restricted compared to 2D and 3D geometries. The beam must be symmetric about the $z$-axis or else it would not actually be a Gaussian beam in the 3D volume of revolution.

Enter the **Beam waist z-coordinate** $z_w$ (SI unit: m). The default is 0. Then, from the **Beam direction** list, select **Positive z-axis** (the default) or **Negative z-axis**.

**BEAM DIMENSIONS**

Select an option from the **Beam type** list:

- **Point source (small Rayleigh range)**, the default, is appropriate when the rays in the model propagate very large distances compared to the beam waist radius or Rayleigh range. The beam waist is treated as a point source, from which rays emanate outward in a cone. The symmetry axis of the cone is the **Beam axis** from the previous section.

- **Collimated source (large Rayleigh range)** is appropriate when the rays propagate for only a short distance compared to the Rayleigh range. The rays are released from a grid of points and initially propagate in the same direction.

*Releasing Rays from a Point Source*

For a **Point source**, enter the **Number of polar angles** $N_\theta$ (dimensionless). The default is 10. In a 2D or 2D axisymmetric geometry, the actual number of rays released is equal to $N_\theta$, while in 3D the total number of rays released is $3N_\theta(N_\theta + 1) + 1$. because rays released at a larger polar angle require a finer sampling of azimuthal angles to ensure uniform sampling within the solid angle subtended by the beam.

To control the width of the beam, select one of the following from the **Beam dimensions** list:

- **Specify beam divergence half-angle** (the default), then enter a value or expression for the **Beam divergence half-angle** $\alpha$ (SI unit: rad). The default is 1 mrad.

- **Specify beam waist radius**, then enter a value or expression for the **Beam waist radius** $w_0$ (SI unit: m). The default is 1 mm. In 2D, this option is instead called **Specify beam waist half-width** and the input is called the **Beam waist half-width** because the

2D beam is uniform in the out-of-plane direction, not rotationally symmetric about the beam axis.

- **Specify Rayleigh range**, then enter a value or expression for the **Rayleigh range** $z_R$ (SI unit: m). The default is 1 mm.

*Releasing Rays from a Collimated Source*

If instead **Collimated source** is selected, enter the **Number of radial positions** $N_c$ (dimensionless) in a 3D or 2D axisymmetric geometry, or the Number of rays per release N (dimensionless). For any dimension, the default is 10. In 3D the total number of rays released is $3N_c(N_c + 1) + 1$ because rays released at greater radial distances from the center of the beam waist require a finer sampling of azimuthal angles, to ensure uniform sampling within the beam cross section. Then enter the **Beam waist radius** $w_0$ (SI unit: m). The default is 1 mm. In 2D this is called the **Beam waist half-width**.

*Beam Cutoff Ratio*

For all of the above settings, enter a value or expression for the **Beam cutoff ratio** $c$ (dimensionless). The default is 1. The cutoff ratio does not affect the other beam parameters but it affects how rays are sampled from the beam.

Theoretically the irradiance and power of light within a Gaussian beam remains nonzero out to an arbitrarily large radial distance. But for practical purposes the beam must be truncated at some point, so that rays will only be released within a finite distance from the center of the beam waist (for collimated sources) or within a finite angle (for point sources).

Changing the value of $c$ changes the maximum distance or angle from the beam axis at which rays are released. For the default value of 1, rays will be released at radial positions out to the waist radius $w_0$ (for a collimated source) or in a cone with angles up to the beam divergence half-angle α (for a point source). In a 3D or 2D axisymmetric beam, the released rays then comprise a fraction of $1 - e^2$ or about 87% of the total beam power. In a 2D sheet beam, this fraction is about 95%.

If the value of $c$ is increased, rays will be released at greater distances from the beam axis (for a collimated beam) or at greater angles (for a point source) and the total power over all of the released rays will be greater than the fractions given above. Setting $c = 2$ results in 99.97% of the total beam power being sampled by the rays. , but most of the released rays will individually have rather low power. At about $c = 4.2$ the released power among all the rays matches the specified total source power to double precision.

## INTENSITY AND POWER

Select one of the following options from the Intensity specification list:

- **Specify total beam power** (the default), then enter a value or expression for the **Total source power** $P_{\mathrm{src}}$ (SI unit: W). The default is 1 W.

- **Specify encircled power**, then enter a value or expression for the **Encircled power** $P_{\mathrm{cir}}$ (SI unit: W). The default is 1 W.

- **Specify Intensity at beam waist**, then enter a value or expression for the **Peak intensity at beam waist** $I_0$ (SI unit: W/m$^2$). The default is 1 W/mm$^2$.

## INITIAL POLARIZATION

This section is a simplified version of the **Initial Polarization** section for the Release node. The main differences are that the **Gaussian Beam** must always release polarized rays, and that the initial polarization direction must be entered directly rather than based on the directions of the principal wavefront curvatures.

- In 3D enter the following:

  - Components of the **Initial polarization reference direction u** (dimensionless). By default the vector points in the positive $y$ direction. This must not be parallel to the beam axis.

  - **Initial polarization parallel to reference direction** $a_{1,0}$ (dimensionless, default 1).

  - **Initial polarization perpendicular to reference direction** $a_{2,0}$ (dimensionless, default 0).

- In 2D axisymmetric models enter the following:

  - **Initial polarization, in plane** $a_{rz,0}$ (dimensionless, default 1)

  - **Initial polarization, out of plane** $a_{\phi,0}$ (dimensionless, default 0).

- In 2D enter the following:

  - **Initial polarization, in plane** $a_{xy,0}$ (dimensionless, default 1)

  - **Initial polarization, out of plane** $a_{z,0}$ (dimensionless, default 0)

For all dimensions, enter the **Initial phase difference** $\delta_0$ (SI unit: rad, default 0).

## VACUUM WAVELENGTH

This section is shown if **Polychromatic, specify vacuum wavelength** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section. Enter a value or expression for the **Vacuum wavelength** $\lambda_0$ (SI unit: m). The default is 660 nm.

This section is shown if **Polychromatic, specify frequency** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section. Enter a value or expression for the **Initial ray frequency** $v_0$ (SI unit: Hz). The default is $4.54 \times 10^{14}$ Hz.

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| | |
|---|---|
| ② | Gaussian Beam Theory |

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## *Illuminated Surface*

Use the **Illuminated Surface** node to release rays under the assumption that the emitted rays are specularly reflected from an external radiation source. It is assumed that the entire selected surface has direct line of sight to the external radiation source; that is, shadowing due to other geometric entities is not taken into account.

See Release for information on the following sections: **Release Times, Initial Ray Frequency**, **Vacuum Wavelength**, **Initial Phase**, **Initial Polarization**, and **Initial Value of Auxiliary Dependent Variables**.

See Release from Boundary for information on the **Initial Position** section.

### RAY DIRECTION VECTOR

Select the **Rays to release**: **Reflected** (the default) or **Refracted**.

- For **Reflected** select the **Reflection coefficient specification**: **Using absorption coefficient** (the default) or **Using refractive indices**.

- For **Refracted** enter a value for **Refractive index of exterior domains** $n_{\text{ext}}$ (dimensionless). The default is $1$. This index is absolute (that is, relative to vacuum).

Select an **Incident ray direction vector**: **User-defined direction** (the default), **User-defined point source**, or **Solar radiation** (3D components only).

Then based on the selection enter the applicable information:

For **User-defined direction** enter the components of the **Incident ray direction vector** $\mathbf{L}_i$ (dimensionless) based on space dimension.

- For **User-defined point source** enter the **Point source location** $\mathbf{r}_{\text{src}}$ (SI unit: m).

- For **Solar radiation** see Solar Radiation for information about the options.

If **User-defined direction** or **Solar radiation** is selected from the **Incident ray direction vector** list, you can include small perturbation factors designed to take the finite size of the sun (or another light source) into account. Select an option from the **Corrections for finite source diameter** list: **None** (the default), **Create light cones at release points**, or **Sample from conical distribution**.

- For **None** no perturbation to the initial ray direction is applied.

- For **Create light cones at release points** a cone-shaped distribution of rays is released at each point. Enter a value for the **Number of rays in wave vector space** (dimensionless) $N_w$ (dimensionless). The default is 50. A cone-shaped distribution containing $N_w$ rays is released at each point, which may cause a very large number of rays to be released.

- For **Sample from conical distribution** a single ray is released at each release point. This ray is given a random perturbation with uniform probability density within a cone-shaped distribution in wave vector space.

For **Create light cones at release points** and **Sample from conical distribution**, specify the **Maximum disc angle** $\Psi_m$ (SI unit: rad). The default is 4.65 mrad, approximately the size of the solar disc when viewed from Earth.

For **Create light cones at release points** and **Sample from conical distribution**, select a **Limb darkening model**: **None** (the default), **Empirical power law**, **Linear**, or **User defined**. The limb darkening model reduces the intensity of solar radiation that is released from the periphery of the solar disk, relative to radiation that is released near the center. For **Linear** enter a **Limb darkening coefficient** $\beta$ (dimensionless). The default value is 0.8. For **User defined** enter a **Limb darkening coefficient** $f_L$ (dimensionless). The default value is 1.

Select the **Include surface roughness** check box to include an additional perturbation term based on uncertainty in the orientation of the surface normal, which is common in imperfect reflecting surfaces. Enter a value or expression for the **Surface slope error** $\sigma$ (SI unit: rad). The default is 1 mrad. The surface normal is then perturbed by a random angle, which is sampled from a Rayleigh distribution.

### INCIDENT RAY INTENSITY

This section is available when the ray intensity is solved for. Enter a value for the **Incident ray intensity** $I_i$ (SI unit: W/m$^2$). The default is 1000 W/m$^2$.

This section is available:

- when the ray intensity is solved for, and

- when **Spherical**, **Hemispherical**, or **Conical** is selected as the **Ray direction vector**.

- It is also available when the ray power is solved for, and then any choice of **Ray direction vector** displays this section.

Enter a **Total source power** $P_{src}$ (SI unit: W). The default is $1$ W. In 2D, instead enter the **Total source power per unit thickness** $P_{src}$ (SI unit: W/m). The default is $1$ W/m.

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| 🔍 | Illuminated Surface Theory |

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| ▥ | The following examples involve buildings or other objects being illuminated by solar radiation in a specific direction:<br><br>• *Solar Dish Receiver*: Application Library path **Ray_Optics_Module/ Solar_Radiation/solar_dish_receiver**<br><br>• *Vdara® Caustic Surface*: Application Library path **Ray_Optics_Module/Solar_Radiation/vdara_caustic_surface** |

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## Solar Radiation

The **Solar Radiation** node uses the solar position to specify the initial direction vector of rays. The node is selected from the **Physics** toolbar, **Global** menu.

See Release for information on the following sections: **Release Times, Initial Ray Frequency**, **Vacuum Wavelength**, **Initial Phase**, and **Initial Value of Auxiliary Dependent Variables**.

### INITIAL COORDINATES

These settings are the same as for the Release from Grid node.

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| 📄 | North, West, and the up directions correspond to the $x$, $y$, and $z$ directions, respectively. |

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Select an option from the **Location defined by** list: **Coordinates** (the default) or **City**.

For **City** select a predefined city and country combination from the list. Click to select the **Include daylight saving time (Time zone + 1)** check box to add one hour to the default setting for the city selected. For example, if **New York City, USA** is selected and the default standard time zone is UTC −5 hours. If the check box is selected, the daylight savings time is used instead (UTC −4 hours). This feature does not automatically deduce whether daylight savings should be applied based on the selected city and date; you must specify it explicitly.

If **Coordinates** is selected, or your city is not listed, in the **Location** table define the:

- **Latitude**, a decimal value, positive in the northern hemisphere (the default is Las Vegas, USA latitude, 36.1). Enter a value without a unit to avoid double conversion. This is because the latitude value is expected to represent degrees but the model's unit for angles may be different (for example, the SI unit for the angle is radians).

- **Longitude**, a decimal value, positive at the East of the Prime Meridian (the default is Las Vegas, USA longitude, −115.2). Enter a value without a unit to avoid double conversion. This is because the latitude value is expected to represent degrees but the model's unit for angles may be different (for example, the SI unit for the angle is radians).

- **Time zone**, the number of hours to add to UTC to get local time (the default is Las Vegas, USA time zone, −8). For example in **New York City, USA** the time zone is UTC −5 hours (standard time zone) or UTC −4 hours (with daylight savings time).

For either selection, in the **Date** table enter the:

- **Day**, the default is 01. Enter a value without a unit to avoid double conversion. This is because the value is expected to represent days but the model's unit for time may be different (for example, the SI unit for time is second).

- **Month**, the default is 10 (October). Enter a value without a unit to avoid double conversion. This is because the value is expected to represent months but the model's unit for time may be different (for example, the SI unit for time is second).

- **Year**, the default is 2014. Enter a value without a unit to avoid double conversion. This is because the value is expected to represent years but the model's unit for time may be different (for example, the SI unit for time is second). The solar position is accurate for a date between 2000 and 2199.

For either selection, in the **Local time** table enter the:

- **Hour**, the default is 12. Enter a value without a unit to avoid double conversion. This is because the value is expected to represent hours but the model's unit for time may be different (for example, the SI unit for time is second).

- **Minute**, the default is 0. Enter a value without a unit to avoid double conversion. This is because the value is expected to represent minutes but the model's unit for time may be different (for example, the SI unit for time is second).

- **Second**, the default is 0.

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The sun position is updated if the location, date, or local time changes during a simulation. Because the time scale of ray propagation is typically many orders of magnitude smaller than the time scale for significant changes in solar position, modeling ray propagation at different times of day typically requires a **Parametric Sweep** over the larger time scale. Note that no validity range is prescribed on the time inputs. It is possible to enter values that exceed the expected boundary. For example, entering 5h 2min 81s is equivalent to 5h 3min 21s. This makes it easier, for example, to run a Parametric Sweep over the time of day using only a single parameter.

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For either selection, in the **Solar irradiance** field $I_s$ (SI unit: $W/m^2$) define the incident radiative intensity coming from the sun.

**ANGULAR PERTURBATIONS**

Select an option from the **Corrections for finite source diameter** list: **None** (the default), **Create light cones at release points**, or **Sample from conical distribution**.

- For **None** no perturbation to the initial ray direction is applied.

- For **Create light cones at release points** a cone-shaped distribution of rays is released at each point. Enter a value for the **Number of rays in wave vector space** (dimensionless) $N_w$ (dimensionless). The default is 50. A cone-shaped distribution containing $N_w$ rays is released at each point, which may cause a very large number of rays to be released.

- For **Sample from conical distribution** a single ray is released at each release point. This ray is given a random perturbation with uniform probability density within a cone-shaped distribution in wave vector space.

For **Create light cones at release points** and **Sample from conical distribution**, specify the **Maximum disc angle** $\Psi_m$ (SI unit: rad). The default is 4.65 mrad.

For **Create light cones at release points** and **Sample from conical distribution**, select a **Limb darkening model**: **None** (the default), **Empirical power law**, **Linear**, or **User defined**. The limb darkening model is typically used to reduce the intensity of solar radiation that is released from the periphery of the solar disk, relative to radiation that is released near the center. For **Linear** enter a **Limb darkening coefficient** β (dimensionless). The default value is 0.8. For **User defined** enter a **Limb darkening coefficient** $f_L$ (dimensionless). The default value is 1.

| | The options for accounting for finite source diameter and solar limb darkening are discussed in the Illuminated Surface Theory section. |
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### *Blackbody Radiation*

| | This feature is only available in 3D. |
|---|---|

The **Blackbody Radiation** node releases rays from selected boundaries with the following properties:

1 The rays are diffusely emitted from one side of the surface, meaning that the initial ray directions are random and their distribution follows Lambert's cosine law,

2 If the Geometrical Optics interface has been set up to trace polychromatic light rays, the vacuum wavelength or frequency of the released rays is random and their distribution follows Planck's Law, and

3 If ray intensity or power is solved for, the total source power is defined using the Stefan-Boltzmann law.

See Release for information on the **Release Times** and **Initial Value of Auxiliary Dependent Variables** sections.

**MODEL INPUT**

Enter a value or expression for the **Temperature** $T$ (SI unit: K), which is used in the Stefan-Boltzmann law for ray power and the Planck equation to sample wavelength or frequency values. The default is 293.15 K. If the temperature has already been solved for in another physics interface, then it may be selected from the list.

Enter an integer value for the **Number of rays per release** $N$ (dimensionless). The default is 1000. The released rays are always randomly distributed over the selected surfaces with uniform probability.

The **Blackbody Radiation** node always releases rays in random directions following Lambert's cosine law, which states that the flux across a differential solid angle element is proportional to the cosine of the angle between that solid angle element and the wall normal direction. While the settings window for the **Blackbody Radiation** node is shown, the orientation of the surface normal is indicated by arrows shown in the Graphics window. You can reverse the direction of the surface normal by selecting or toggling the **Reverse direction** check box.

<div align="center">🔍     Blackbody Radiation Theory</div>

*Ray Termination*

Use the **Ray Termination** feature to remove rays from the model as they exit the geometry, or to annihilate rays of sufficiently low intensity or power. Only one **Ray Termination** node can be added to the model, but it is possible to combine position-based and intensity-based criteria for removing rays if the ray intensity or power is computed by the model.

**TERMINATION CRITERIA**
Select an option from the **Spatial extents of ray propagation** list: **Bounding box, from geometry** (the default), **Bounding box, user defined**, or **None**. This list controls whether rays are terminated based on their positions.

- For **Bounding box, from geometry**, a ray is immediately terminated if it reaches the surface of the bounding box of the geometry, defined as the smallest rectangle or rectangular prism with edges parallel to the axes of the global coordinate system that encloses all of the geometric entities. This bounding box is extended by 5% in each direction so that rays can still interact with boundaries that coincide with the perimeter of the bounding box. Therefore rays can propagate a short distance away from the geometry before disappearing.

- For **Bounding box, user defined**, a ray is immediately terminated if it reaches the surface of a box of user-specified dimensions. To define the box, enter maximum and minimum values of each spatial coordinate.

- For **None**, the rays that propagate outward from the geometry will continue to propagate until the study is complete. If the maximum path length for the **Ray Tracing** study step is too large, this may result in trajectories that are extremely long relative to the characteristic geometry size.

If rays are released from outside the bounding box, they will not immediately disappear; instead, they will only disappear if they enter the bounding box and then exit it again.

*Intensity- and Power-Based Termination Criteria*
If the ray intensity or power is being computed in the model, you can then terminate rays based on either or both of these quantities.

Select an option from the **Additional termination criteria** list. **None** (the default) is always available. If ray intensity is solved for, then **Intensity** is available. If ray power is solved for, then **Power** is available. If both ray intensity and power are solved for, the **Intensity and Power** option is also shown.

- For **Intensity** or **Intensity and power**, enter the **Threshold intensity** $I_{th}$ (SI unit: W/m$^2$). The default is $1$ mW/m$^2$. Rays will be removed from the model if their intensity decreases below the specified value.

- For **Power** or **Intensity and power**, enter the **Threshold power** $Q_{th}$ (SI unit: W). The default is $10^{-3}$ mW.

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| | The **Ray Termination** feature can terminate rays at the exact time at which their intensity or power reaches the specified threshold (to within numerical precision), if there exists a closed-form analytic expression for this time. Such a closed-form analytic solution exists if: |
|---|---|
| | • The rays represent planar wavefronts in an absorbing medium, or |
| | • The rays represent spherical or ellipsoidal wavefronts in a nonabsorbing medium. |
| | Otherwise, the rays are stopped at the first discrete time step taken by the solver for which the intensity or power is less than the threshold value. |

*Scattering Domain*

Use the **Scattering Domain** feature to model extinction of light by a medium containing a number of small spherical particles. As rays propagate through the selected domains, some energy is either converted into heat within the particles (absorption) or sent in a different direction (scattering). The overall removal of light from the initial beam propagation direction is called extinction.

### SCATTERING MODEL

The **Scattering model** list is only shown if the ray intensity or power is solved for. If so, choose either **Deterministic** or **Random** (the default). If ray intensity or power is not solved for, this feature always behaves as if **Random** is selected.

- If **Deterministic** is selected, the ray intensity and power will continuously decrease as rays propagate through the selected domains, but the total number or rays will remain the same. If the number density and size of the scattering particles is spatially uniform, the intensity and power will decay exponentially.

- If **Random** is selected, rays will have some probability of disappearing as they propagate through the selected domains. If the ray intensity and power are solved for, they will not continuously decrease along the ray trajectories.

Use the **Deterministic** option for a reproducible result where nothing is random and the ray variables vary continuously; the **Random** option is more of a Monte Carlo approach.

Choose an option from the **Cross section calculation** list. The correct choice depends on the size of the scattering particles in comparison with the wavelength. The individual scattering particles are said to be optically large if the particle diameter is much larger than the wavelength of the radiation. The following options are available:

- **Small spheres (Rayleigh theory)** (the default) is an approximate solution for optically small particles. The particle must be much smaller than the wavelength both inside and outside the particle, an important consideration for tiny metallic particles.

- **General spheres (Mie theory)** is a full solution to the electromagnetic wave equation as a plane wave interacts with a sphere. It is the most accurate solution across a wide range of optical sizes, and the only approach that gives excellent accuracy at

intermediate optical sizes, when the wavelength and particle diameter are similar in size. The calculation becomes more time-consuming for extremely large particles.

- **Large conducting spheres (isotropic reflection)** represents the asymptotic limit of scattering by spheres much larger than the wavelength. The total extinction cross section is double the geometrical cross section of the sphere because the sphere blocks a certain amount of light and also causes diffraction along its perimeter.

- If **Specify efficiency factors** is selected, enter values or expressions for the dimensionless extinction and scattering efficiency factors.

- If **Specify cross section** is selected, enter values of expressions for the scattering and absorption cross sections directly.

For all choices of **Cross section calculation** except **Specify cross section**, enter the **Radius of scattering particle** $R$ (SI unit: m). The default is 1 μm.

For all choices of **Cross section calculation**, enter the **Number density of scattering particles** $N$ (SI unit: $1/m^3$). The default is $10^{20}$ m$^{-3}$.

If **Small spheres (Rayleigh theory)** or **General spheres (Mie theory)** is selected, enter the **Particle refractive index, real part** $n_{p,r}$ (dimensionless). The default is 1.4. Also enter the **Particle refractive index, imaginary part** $n_{p,i}$ (dimensionless). The default is $10^{-6}$. Internally the complex-valued refractive index is defined as $n = n_{p,r} - in_{p,i}$, so positive values here indicate that the scattering particle is absorbing.

If **Specify efficiency factors** is selected, enter the **Extinction efficiency** $Q_{ext}$ (dimensionless). The default is 2. Also enter the **Scattering efficiency** $Q_{sca}$ (dimensionless). The default is 2. The absorption efficiency $Q_{abs}$ is then the difference between the extinction efficiency and the scattering efficiency.

If **Specify cross section** is selected, enter the **Extinction cross section** $\sigma_{ext}$ (SI unit: m$^2$). The default is $10^{-15}$ m$^2$. Also enter the **Scattering cross section** $\sigma_{sca}$ (SI unit: m$^2$). The default is $10^{-15}$ m$^2$. The absorption cross section $\sigma_{abs}$ is then the difference between the extinction cross section and the scattering cross section. The scattering efficiency (cross section) should not be greater than the extinction efficiency (cross section).

Q    Volumetric Scattering Theory

*Scattering Boundary*

The scattering boundary can be used to scatter rays in reflection and transmission from any boundary using one of several scattering models:

- **Diffuse scattering** will scatter rays according to Lambert's cosine law. That is, the probability of a ray propagating in a given direction within a solid angle $d\omega$ is given by $\cos\theta\, d\omega$ where $\theta$ is the angle between the direction of the ray and the wall normal.

- **Isotropic scattering** will cause rays to be randomly scattered in all directions.

- **Surface slope error** will cause the surface normal to be perturbed by a random angle sampled from a Rayleigh distribution based on the value or expression for the **Surface slope error** $\sigma$ (SI unit: rad). The default is 1 mrad.

Rays can be released from a **Scattering Boundary** in both reflection and transmission. That is, the options for which **Rays to release** include **Reflected and transmitted** (the default), **Reflected**, or **Transmitted**.

If both reflected and transmitted rays are chosen, then, unless total internal reflections occurs, the primary rays are expected to be transmitted.

### WAVELENGTH OR FREQUENCY REINITIALIZATION

This section is available when the distribution of released rays is either **Polychromatic, specify vacuum wavelength**, or **Polychromatic, specify frequency**. If activated the wavelength or frequency of a ray can be reset as it interacts with the selected boundaries. The new wavelength or frequency distribution function can be:

- **None** – the wavelength or frequency is set to a user defined expression.

- **Normal** – the wavelength or frequency distribution will follow a normal (Gaussian) distribution with a user defined **Mean vacuum wavelength** or **Mean frequency** $\mu$, and a **Vacuum wavelength standard deviation** or **Frequency standard deviation** $\sigma$.

- **Lognormal** – the wavelength or frequency distribution will follow a log normal (Gaussian) distribution with a user defined **Mean vacuum wavelength** or **Mean frequency** $\mu$, and a **Vacuum wavelength standard deviation** or **Frequency standard deviation** $\sigma$

- **Uniform** – the wavelength or frequency will be drawn from interval specified by the **Minimum vacuum wavelength** $\lambda_{0,min}$ or **Minimum frequency** $\nu_{min}$ and the **Maximum vacuum wavelength** $\lambda_{0,max}$ or **Maximum frequency** $\nu_{max}$

**NEW VALUES OF AUXILIARY DEPENDENT VARIABLES**

See Wall for information on the section **New Value of Auxiliary Dependent Variables.**

**ADVANCED SETTINGS**

All of the scattering models (and wavelength or frequency reinitialization) generate random numbers. The option to enter an **Additional input argument to random number generator** $i$ (dimensionless, default 1) is possible if in the **Advance Settings** section for the Geometrical Optics interface, the **Arguments for random number generation** setting is set to **User defined**. The **Advanced Settings** section is also shown if the **Compute optical path length** check box is selected under the physics interface **Additional Variables** section. Select the **Reset optical path length** check box to set the optical path length to 0 when a ray interacts with a scattering boundary.

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> ❓  Surface Scattering Theory

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*Release from Electric Field*

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> 📋  This feature is only available if the ray intensity or power is solved for. Select an appropriate option from the **Intensity computation** list in the physics interface **Intensity Computation** section.

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Use the **Release from Electric Field** node to release rays from selected boundaries, with initial intensity and polarization based on the incident electric field at that boundary. The electric field may be user defined or solved for in a previous study.

See Release for information on the **Initial Values of Auxiliary Dependent Variables** section and the optional **Release Times** section. See Release from Boundary for information on the **Initial Position** section.

**RAY DIRECTION VECTOR**

Select an option from the Ray direction vector list: **Parallel to Poynting vector**, **Outward normal** (the default), or **Inward normal**. For **Outward normal** and **Inward normal** the direction of the released rays is indicated by an arrow in the Graphics window.

The **Parallel to Poynting vector** option can be useful when the outgoing wave makes an oblique angle with an absorbing boundary, such as a **Port**, **Scattering Boundary Condition**, or **Matched Boundary Condition**; or when the simulation domain is

surrounded by a **Perfectly Matched Layer**. In those scenarios, releasing the rays normal to the surface might not be accurate.

> ⚠ For the **Parallel to Poynting vector** option, it is not sufficient to only know the electric field at the surface; it must be differentiable in both the tangential and normal directions. Usually this means that selecting an **Electric field** defined by one of the Electromagnetic Waves interfaces will work, but selecting a **Tangential electric field** will fail.

### INCIDENT ELECTRIC FIELD

Enter values or expressions in the table for the **Electric field E** (SI unit: V/m) based on space dimension. If the electric field is computed by another physics interface then it can be selected from the list.

The **Use frequency from the coupled physics interface as the ray frequency** check box is cleared by default. If this check box is cleared, the wavelength or frequency of the released rays may be specified depending on the option selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section:

- If **Polychromatic, specify vacuum wavelength** is selected, enter the **Vacuum wavelength** $\lambda_0$ (SI unit: m). The default is 660 nm.
- If **Polychromatic, specify frequency** is selected, enter the **Ray frequency** ν (SI unit: $1/$ s). The default is $4.54 \times 10^{14}$ Hz.

If this check box is selected, then the frequency or wavelength of the released rays will be determined by the **Frequency Domain** or **Wavelength Domain** study in the **Values of Variables not Solved For** section of the **Time Dependent** solver settings. Typically this **Frequency Domain** or **Wavelength Domain** study would first be used to solve for the electric field, using either the Electromagnetic Waves, Frequency Domain interface or the Electromagnetic Waves, Beam Envelopes interface.

Selecting this check box may also cause the frequency or wavelength specified in the Ray Properties node to be ignored while the **Release from Electric Field** node is active.

> ⚲ In the Geometrical Optics interface, ray intensity is stored in the Stokes parameters for each ray. For more information, see Intensity, Wavefront Curvature, and Polarization in Theory for the Geometrical Optics Interface.

|     | *Ray Release Based on a Plane Electromagnetic Wave*: Application Library path **Ray_Optics_Module/Tutorials/plane_em_wave_to_ray_release** |
| --- | --- |

*Release from Far-Field Radiation Pattern*

|     | This feature requires at least one of the following licenses: RF Module, Wave Optics Module. |
| --- | --- |
|     | In addition, this feature is only available if the ray intensity or power is solved for. Select an appropriate option from the **Intensity computation** list in the physics interface **Intensity Computation** section. |

Use the **Release from Far-Field Radiation Pattern** node to release rays with an intensity and power distribution based on a far-field radiation pattern. The far-field radiation pattern must first be solved for in a previous study.

The **Release from Far-Field Radiation Pattern** node can be used for multiscale electromagnetics modeling. First, the Electromagnetic Waves, Frequency Domain interface should be used to compute the electric field in the immediate vicinity of a radiation source, such as an antenna or waveguide. The **Far-Field Domain** node and its default subnode, **Far-Field Calculation**, should be added to this instance of the Electromagnetic Waves, Frequency Domain interface. In this wavelength-scale model, the mesh must be fine enough to resolve individual oscillations of the electric field, fulfilling the *Nyquist criterion*. Typically this requires 10 linear elements or 5 second-order elements per wavelength.

Then, in the same model component or a different component, the Geometrical Optics interface can be used to extend the far field over an arbitrarily large number of wavelengths, because the ray tracing approach does not require a finite element mesh fine enough to resolve individual oscillations of the electric field.

The **Release from Far-Field Radiation Pattern** node is only available in 3D. However, the far-field function used to initialize the ray intensity and polarization can be defined either in a 3D model component or a 2D axisymmetric model component. If the previous model component was a 2D axisymmetric component, the intensity distribution of released rays will also be assumed to be axisymmetric.

See Release for information on the **Initial Values of Auxiliary Dependent Variables** section and the optional **Release Times** section.

### INITIAL COORDINATES

Select an option from the **Grid type** list: **All combinations** (the default) or **Specified combinations**.

*Linear, Rectangular, and Arbitrary Grids*

Enter **Initial coordinates** based on space dimension ($q_{x,0}$, $q_{y,0}$, and $q_{z,0}$) for the ray positions or click the **Range** button (  ) to select and define a range of specific coordinates.

If **Specified combinations** is selected, the number of initial coordinates entered for each space dimension must be equal, and the total number of rays released is equal to the length of one of the lists of initial coordinates. If **All combinations** is selected, the total number of rays released is equal to the product of the lengths of each list of initial coordinates.

*Previewing Grid Points*

In the **Initial Coordinates** section, you can click the **Preview Initial Coordinates** and **Preview Initial Extents** buttons to visualize the ray release positions. Clicking **Preview Initial Coordinates** will cause a point to appear in the Graphics window for every release position. Clicking **Preview Initial Extents** will cause a bounding box to appear, indicating the spatial extents of the released rays.

### RAY DIRECTION VECTOR

Select an option from the **Ray direction vector** list: **Spherical** (the default), **Hemispherical**, or **Conical**.

- For **Spherical** a number of rays are released at each point, sampled from a spherical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50.

- For **Hemispherical** a number of rays are released at each point, sampled from a hemispherical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then select an option from the **Hemisphere axis** list: **From Euler angles** or **User Defined**. For **User Defined** enter coordinates for the **Hemisphere axis r** based on space dimension.

- For **Conical** a number of rays are released at each point, sampled from a conical distribution in wave vector space. Enter the **Number of rays in wave vector space** $N_w$ (dimensionless). The default is 50. Then select an option from the **Cone axis** list: **From Euler angles** or **User Defined**. For **User Defined** enter coordinates for the **Cone axis r** based on space dimension. Then enter the **Cone angle** $\alpha$ (SI unit: rad). The default is $\pi/3$ radians.

Note that unlike the Release from Grid feature, the options **Expression** and **Lambertian** are not available here. In addition, if **Conical** is selected, the cone must be isotropic. This is because each ray is assumed to subtend approximately the same solid angle, so direction distributions that give unequal weight to some directions (like **Lambertian**) or options with no direction distribution at all (like **Expression**) cannot initialize the ray intensity and power in a consistent and physically meaningful way.

### FAR-FIELD VARIABLE NAME

Enter an expression for the **Far-field variable name**. The default expression is Efar. This expression must match the variable name in a corresponding **Far-Field Calculation** feature.

### SOURCE ORIENTATION

Use the settings in this section to orient the ray source. This allows, for example, the release of rays from an antenna to be modeled with the antenna oriented in many different directions, while only solving for the far-field radiation pattern once.

Enter the **Euler angles (Z-X-Z)**. The labels Z-X-Z indicate the order in which rotation about the different axes is performed. First, the local coordinate system of the radiation pattern is rotated about its *Z*-axis by the angle $\alpha$. Then it is rotated about its *X*-axis (which is now at an angle $\alpha$ to the global *x*-axis) by the angle $\beta$. Finally, this local coordinate system is rotated about its new *Z*-axis by the angle $\gamma$. All three inputs are plane angles (SI unit: rad) with default values of 0.

### ADVANCED SETTINGS

This section is only shown if **Monochromatic** is selected from the **Wavelength distribution of released rays** list in the physics interface **Ray Release and Propagation** section.

The **Use frequency from the far-field calculation as the ray frequency** check box is selected by default. While this check box is selected and the **Release from Far-Field Radiation Pattern** feature is active, the frequency or vacuum wavelength of released rays will be determined by the **Frequency Domain** or **Wavelength Domain** study in the **Values of Variables not Solved For** section of the **Time Dependent** solver settings. Usually, this previous study was used to solve for the far-field radiation pattern using the Electromagnetic Waves, Frequency Domain interface.

While this check box is selected and the **Release from Far-Field Radiation Pattern** node is active, the frequency or wavelength specified in the Ray Properties node is ignored.

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|---|---|
| Q | In the Geometrical Optics interface, ray intensity is stored in the Stokes parameters for each ray. For more information, see Intensity, Wavefront Curvature, and Polarization in the theory section. |

| | |
|---|---|
| ▥ | *Ray Release from a Dipole Antenna Source (3D)*: Application Library path **Ray_Optics_Module/Tutorials/ ray_release_from_dipole_antenna_source_3d** |
| | *Ray Release from a Dipole Antenna Source (2D Axisymmetric)*: Application Library path **Ray_Optics_Module/Tutorials/ ray_release_from_dipole_antenna_source_2daxi** |

## *Grating*

Use the **Grating** node to treat a boundary as a diffraction grating that can release reflected and transmitted rays into multiple diffraction orders. A Diffraction Order (Grating) subnode for reflected and transmitted rays of order $m = 0$ is added by default. Change the settings for this default subnode to release rays of a different diffraction order. You can also release rays of multiple diffraction orders from the same boundary by adding more **Diffraction Order** subnodes from the from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

The Accumulator (Boundary) subnode is also available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### *Releasing Secondary Rays*
When two or more rays are released from a **Grating** boundary, one of the released rays uses the same degrees of freedom as the incident ray. The remaining degrees of freedom must be preallocated in memory as secondary rays. The total number of secondary rays that can be released in the model is controlled by the **Maximum number of secondary rays** field in the physics interface **Ray Release and Propagation** section.

For example, if both reflected and transmitted rays of diffraction orders $m = -1$, $m = 0$, and $m = 1$ are released from a boundary, then for every incident ray, a total of five secondary rays are released. If the diffraction order $m = -1$ is the first subnode to appear in the Model Builder, then the transmitted ray of order $m = -1$ uses the same

degree of freedom as the incident ray, and the other rays are secondary rays. If the **Maximum number of secondary rays** is 500 and more than 100 rays interact with the grating, then no more secondary rays are emitted and a warning is generated by the solver, indicating that the **Maximum number of secondary rays** should be increased.

### DEVICE PROPERTIES

Select an option from the **Rays to release** list: **Reflected and transmitted** (the default), **Reflected**, or **Transmitted**. This setting affects the release of rays of all diffraction orders.

Enter the a **Grating constant** $d$ (SI unit: m), which is the distance between consecutive lines in the grating, that is, the length of one unit cell. The default is 5 µm. Then select an option from the **Interpretation of grating constant** list: **Unit cell width on surface** (the default) or **Projected unit cell width**.

> ⚠️ The choice of **Interpretation of grating constant** is particularly important for curved diffraction gratings.

- If **Unit cell width on surface** is selected, the value of $d$ is just the distance from one unit cell to the next in a direction tangent to the selected surface.
- If **Projected unit cell width** is selected, enter the components of the **Projection direction** $\mathbf{n}_p$ (dimensionless). The default is the positive $y$ direction in 2D or the positive $z$ direction in 3D. Then the specified **Grating constant** is interpreted as the distance between the projections of grating grooves onto a tangent plane with a surface normal in the direction of $\mathbf{n}_p$. If $d$ represents the projected unit cell spacing, then the actual cell spacing in the direction tangent to the surface is $d/\cos\phi$, where $\phi$ is the angle between the projection direction and the surface normal.

Select **Use relative order numbers** if the grating blaze angle is known, and diffraction into the highest-efficiency orders is desired. Then enter the **Grating blaze angle** $\theta_B$ (SI unit: rad). The default is 0. The absolute order number will be computed based on the blaze angle and the refractive indices of the adjacent domains.

If **Use relative order numbers** is not selected, then the **Automatic Diffraction Order Calculation** section will be present. This will be discussed below.

If the ray power is solved for, the **Store total transmitted power** and **Store total reflected power** check boxes are shown. Select them to declare auxiliary dependent variables for the total power of all transmitted and reflected diffraction orders, respectively.

**GRATING ORIENTATION**

In 2D, select an option from the **Direction of periodicity** list: **Forward** (the default) or **Reverse**. For either setting, an arrow appears in the Graphics window, lying tangent to the selected edges. Reflected and refracted rays from positive diffraction orders have a larger ray direction component in the direction of this arrow, compared to rays from negative diffraction orders.

In 3D, select an option from the **Grating orientation list**: **Specify direction of periodicity** (the default) or **Specify direction of grating lines**.

- If **Specify direction of periodicity** is selected, select an option from the **Direction of periodicity** list: **User defined** (the default) or **Parallel to reference edge**. For **User defined** enter the components of the direction of periodicity $\mathbf{T}_p$ (dimensionless) directly. The default is the positive $x$-axis. For **Parallel to reference edge**, the **Reference Edge Selection** section is shown in the Settings window. Select a single edge, which must be adjacent to at least one boundary in the selection for the **Grating** feature.

- If **Specify direction of grating lines** is selected, select an option from the **Direction of grating lines** list: **User defined** (the default) or **Parallel to reference edge**. For **User defined** enter the components of the direction of grating lines $\mathbf{T}_l$ (dimensionless) directly. The default is the positive $y$-axis. For **Parallel to reference edge**, the **Reference Edge Selection** section is shown in the Settings window. Select a single edge, which must be adjacent to at least one boundary in the selection for the **Grating** feature.

Regardless of how $\mathbf{T}_p$ or $\mathbf{T}_l$ has been specified, the direction of periodicity projected onto the grating surface $\mathbf{T}_g$ will be computed. This is shown in Figure 3-8 for 2D and Figure 3-9 for 3D.
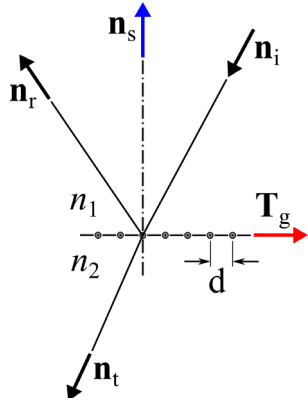


Figure 3-8: Diagram of diffraction grating orientation in 2D.
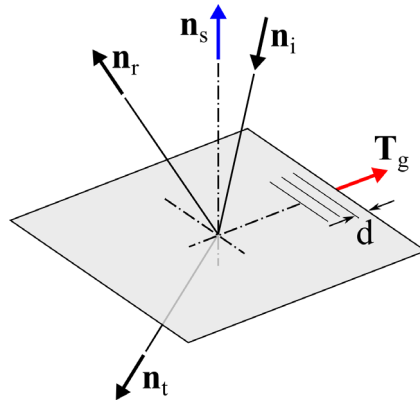


Figure 3-9: Diagram illustrating the options to specify grating orientation in 3D.

AUTOMATIC DIFFRACTION ORDER CALCULATION

> The **Automatic Diffraction Order Calculation** section is not shown if the **Use relative order numbers** check box is selected; see the **Device Properties** section.

Use the **Add Diffraction Orders** button to automatically add diffraction orders to the **Grating** feature. The other settings in this section allow you to automatically generate

the diffraction orders that would be produced by a ray of specified wavelength at a specified angle of incidence. The recommended workflow is to first configure all of the inputs in this section, and then click **Add Diffraction Orders**.

For each diffraction order a corresponding Diffraction Order (Grating) subnode will be added to this node. If some **Diffraction Order** subnodes are already present, then clicking **Add Diffraction Orders** will delete them and replace them with the automatically generated nodes. A warning will be issued if this operation might result in the creation of a very large number of subnodes.

From the **Automatic diffraction order type** list select either **Specify minimum wavelength** (the default) or **Specify maximum frequency.** The **Minimum wavelength** or **Maximum frequency** can be either taken **From Physics** (the default) or **User defined**. If **From Physics** is selected, then the algorithm that generates the diffraction orders will first search through all ray release features to determine the minimum wavelength.

In addition, specify the **Angle of incidence** $\theta_i$ (SI unit: rad). In 3D, instead enter both the **Angle of incidence, in plane** $\theta_{i,in}$ (SI unit: rad) and the **Angle of incidence, out of plane** $\theta_{i,out}$ (SI unit: rad). Also enter the **Refractive index, incoming** $n_1$ and **Refractive index, outgoing** $n_2$. The defaults are 0. If the **Rays to release** are **Reflected** then $n_2 = n_1$. See Figure 3-10 and Figure 3-11 for details.
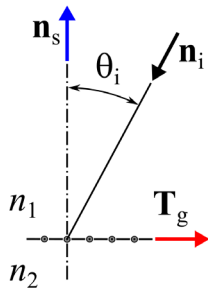


*Figure 3-10: The definition of the angle of incidence in 2D.*
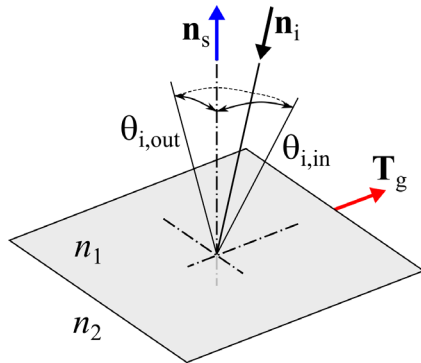
*Figure 3-11: The definition of the in-plane and out-of-plane angles of incidence in 3D.*

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🔍 | Diffraction Grating Theory

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## Diffraction Order (Grating)

The **Diffraction Order** subnode is available from the context menu (right-click the Grating parent node) or from the **Physics** toolbar, **Attributes** menu. Each **Diffraction Order** subnode can either release transmitted rays, reflected rays, or both transmitted and reflected rays of a specified diffraction order, depending on the option selected from the **Rays to release** list in the parent **Grating** node.

### DEVICE PROPERTIES

If the **Use relative order numbers** is not selected in the settings for the parent **Grating** node, then enter a **Diffraction order** $m$ (dimensionless). The default is $m = 0$ for the first **Diffraction Order** added. When more diffraction orders are added to the model, the new default is the highest diffraction order currently present, plus 1.

If **Use relative order numbers** is selected in the settings for the parent **Grating** node, then enter a **Relative diffraction order** $\Delta m$ (dimensionless). As above, the default is $\Delta m = 0$ if no other **Diffraction Order** subnode exists; otherwise the default is 1 greater than the highest relative order that is currently present.

When the ray intensity or power is solved for, enter the **Reflectance** $R$ and the **Transmittance** $T$ (both dimensionless). If the reflectance or transmittance of a certain diffraction order is exactly zero, that diffraction order will not be released.

This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Material Discontinuity feature.

**AUXILIARY DEPENDENT VARIABLES, REFLECTED RAY**

This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Material Discontinuity feature.

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If relative order numbers are being used then the absolute order number can be tracked using an auxiliary dependent variable.

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*Cross Grating*

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This feature is only available in 3D.

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Use the **Cross Grating** node to treat a boundary as a diffraction grating that can release reflected and transmitted rays into multiple diffraction orders. Unlike a standard Grating, a **Cross Grating** can have two directions of periodicity; the boundary is treated as a general two-dimensional periodic substructure. A Diffraction Order (Cross Grating) subnode for reflected and transmitted rays in order $m = n = 0$ is added by default. Change the settings for this default subnode to release rays into different diffraction orders. You can also release rays of multiple diffraction order pairs from the same boundary by adding more **Diffraction Order** subnodes from the from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

The Accumulator (Boundary) subnode is also available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

*Releasing Secondary Rays*
When two or more rays are released from a **Cross Grating** boundary, one of the released rays uses the same degrees of freedom as the incident ray. The remaining degrees of freedom must be preallocated in memory as secondary rays. The total number of secondary rays that can be released in the model is controlled by the **Maximum number of secondary rays** field in the physics interface **Ray Release and Propagation** section. See the Grating feature for further details.

Select an option from the **Rays to release** list: **Reflected and transmitted** (the default), **Reflected**, or **Transmitted**. Then enter the **Grating constant, direction 1** $d_1$ (SI unit: m) and the **Grating constant, direction 2** $d_2$ (SI unit: m). The defaults are $d_1 = 1$ µm and $d_2 = 2$ µm.

If the ray power is solved for, the **Store total transmitted power** and **Store total reflected power** check boxes are shown. Select them to declare auxiliary dependent variables for the total power of all transmitted and reflected diffraction orders, respectively.

**GRATING ORIENTATION**

The **Cross Grating** requires two grating orientations to be specified. For each of **Grating orientation 1** and **Grating orientation 2** select either **Specify direction of periodicity** (the default) or **Specify direction of grating lines**. The **Grating orientation 2** may also be **Orthogonal to grating orientation 1**.

- If **Specify direction of periodicity** is selected, select an option from the **Direction of periodicity 1** (or **2**) list: **User defined** (the default) or **Parallel to reference edge**. For **User defined** enter the components of the direction of periodicity $\mathbf{T}_{p,1}$ or $\mathbf{T}_{p,2}$ (dimensionless) directly. The defaults for $\mathbf{T}_{p,1}$ and $\mathbf{T}_{p,2}$ are the positive $x$-axis and positive $y$-axis respectively. For **Parallel to reference edge**, the **Reference Edge Selection, Direction 1** and/or **Reference Edge Selection, Direction 2** sections are shown. Select a single edge (for each direction), which must be adjacent to at least one boundary in the selection for the **Cross Grating** feature and not parallel to each other.

- If **Specify direction of grating lines** is selected, select an option from the **Direction of grating lines 1 (or 2)** list: **User defined** (the default) or **Parallel to reference edge**. For **User defined** enter the components of the direction of grating lines $\mathbf{T}_{l,1}$ or $\mathbf{T}_{l,2}$ (dimensionless) directly. The defaults for $\mathbf{T}_{l,1}$ and $\mathbf{T}_{l,2}$ are the positive $y$-axis and positive $x$-axis respectively. For **Parallel to reference edge**, the **Reference Edge Selection, Direction 1** and/or **Reference Edge Selection, Direction 2** sections are shown. Select a single edge (for each direction), which must be adjacent to at least one boundary in the selection for the **Cross Grating** feature and not parallel to each other.

Similar to the Grating, regardless of the grating orientations are specified, the directions of periodicity projected onto the grating surface $\mathbf{T}_{g,1}$ and $\mathbf{T}_{g,2}$ will be computed. This is shown in Figure 3-12, along with typical paths for incident reflected, and transmitted rays.
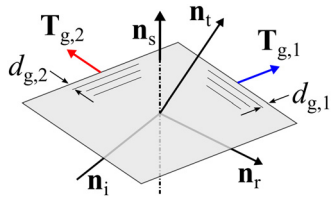
*Figure 3-12: Diagram illustrating the cross grating orientation. The directions of periodicity and/or lines (which need not be orthogonal) are projected onto the cross grating surface.*

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🔍      Diffraction Grating Theory

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## *Diffraction Order (Cross Grating)*

The **Diffraction Order** subnode is available from the context menu (right-click the Cross Grating parent node) or from the **Physics** toolbar, **Attributes** menu. Each **Diffraction Order** subnode can either release transmitted rays, reflected rays, or both transmitted and reflected rays of the specified order, depending on the option selected from the **Rays to release** list in the parent **Cross Grating** node.

### DEVICE PROPERTIES

Enter the **Diffraction orders** $m$ and $n$ (dimensionless). The default is $m = n = 0$ for the first **Diffraction Order** subnode added. When more diffraction orders are added to the model, the new default created by adding 1 to either $m$ or $n$, whichever is lowest. If $m$ and $n$ are equal, then $m$ is incremented by 1.

When the ray intensity or power is solved for, enter the **Reflectance** $R$ and the **Transmittance** $T$ (both dimensionless). If the reflectance or transmittance of a certain diffraction order is exactly zero, that diffraction order will not be released.

### AUXILIARY DEPENDENT VARIABLES, REFRACTED RAY

This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Material Discontinuity feature.

### AUXILIARY DEPENDENT VARIABLES, REFLECTED RAY

This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Material Discontinuity feature

## Linear Polarizer

Use the **Linear Polarizer** node to define a linear polarizer on a boundary selection. Add this node from the **Optical Devices** submenu when ray intensity or power is solved for in the model. The Accumulator (Boundary) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### DEVICE PROPERTIES
Select a **Transmission axis specification**:

- **User defined** (the default). Then enter coordinates for the **Transmission axis T** (dimensionless).
- **Parallel to reference edge** (for 3D components). The **Reference Edge Selection** section is then shown. Add an edge to this selection to specify the transmission axis orientation. Only a single edge may be selected. The edge must be adjacent to a boundary in the physics feature selection.
- **In-plane** or **Out-of-plane** (for 2D and 2D axisymmetric components)

### NEW VALUE OF AUXILIARY DEPENDENT VARIABLES
This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Wall feature.

|     |     |
| --- | --- |
| ② | Linear Polarizer Theory |

## Ideal Depolarizer

Use the **Ideal Depolarizer** node to reinitialize the Stokes parameters so that the outgoing ray is completely unpolarized. Add this node from the **Optical Devices** submenu when ray intensity or power is solved for in the model. The Accumulator (Boundary) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

This section is available if an Auxiliary Dependent Variable has been added to the model.

| 🔍 | Ideal Depolarizer Theory |

## *Linear Wave Retarder*

Use the **Linear Wave Retarder** node to define a linear wave retarder on a boundary selection. Add this node from the **Optical Devices** submenu when ray intensity or power is solved for in the model. The Accumulator (Boundary) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### DEVICE PROPERTIES

Select a **Fast axis specification**:

- **User defined** (the default). Then enter coordinates for the **Fast axis F** (dimensionless).
- **Parallel to reference edge** (for 3D components). The **Reference Edge Selection** section is then shown. Add an edge to this selection to specify the fast axis orientation. Only a single edge may be selected. The edge must be adjacent to a boundary in the physics feature selection.
- **In-plane** or **Out-of-plane** (for 2D and 2D axisymmetric components)

For any selection, enter a value for the **Retardance** $\delta$ (SI unit: rad).

### NEW VALUE OF AUXILIARY DEPENDENT VARIABLES

This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Wall feature.

| 🔍 | Linear Wave Retarder Theory |

## Circular Wave Retarder

Use the **Circular Wave Retarder** node to define a circular wave retarder on a boundary selection. Add this node from the **Optical Devices** submenu when ray intensity or power is solved for in the model. The Accumulator (Boundary) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### DEVICE PROPERTIES

Enter a value for the **Retardance** $\delta$ (SI unit: rad).

By default the **Sense of rotation depends on ray trajectory** check box is not selected. This means a positive value of the retardance always corresponds to clockwise rotation of the polarization ellipse. Select the check box then a positive value of the retardance corresponds to clockwise rotation of the polarization ellipse only when the ray crosses the boundary in the direction indicated by the normal vector in the Graphics window.

The **Reverse sense of rotation** check box is available when the **Sense of rotation depends on ray trajectory** check box is selected. Click to select this check box to reverse the direction of the normal vector shown in the Graphics window.

### NEW VALUE OF AUXILIARY DEPENDENT VARIABLES

This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Wall feature.

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> ⊕   Circular Wave Retarder Theory

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## Mueller Matrix

Use the **Mueller Matrix** node to define Mueller matrices for customized optical components. Add this node from the **Optical Devices** submenu when ray intensity or power is solved for in the model. The Accumulator (Boundary) subnode is available from the context menu (right-click the parent node) or from the **Physics** toolbar, **Attributes** menu.

### DEVICE PROPERTIES

Select a **Reference axis specification**:

• **User defined** (default). Enter coordinates for the **Reference axis** $\mathbf{R}$ (dimensionless).

- **Parallel to reference edge** (for 3D components). The **Reference Edge Selection** section is then shown. Add an edge to this selection to specify the reference direction orientation. Only a single edge may be selected. The edge must be adjacent to a boundary in the physics feature selection.
- **In-plane** or **Out-of-plane** (for 2D and 2D axisymmetric components).

For any choice, select **Isotropic** (the default), **Diagonal**, **Symmetric**, or **Full** from the list. Then enter a value or expression for the **Mueller matrix M** in the matrix or field.

### NEW VALUE OF AUXILIARY DEPENDENT VARIABLES

This section is available if an Auxiliary Dependent Variable has been added to the model. The settings are the same as for the Wall feature.

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Q    Theory of Mueller Matrices and Optical Components

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## *Fluence Rate Calculation*

The **Fluence Rate Calculation** node is used to compute the fluence rate within domains. Fluence rate is defined as the total radiant power that would hit a small sphere located within the domain, divided by the cross sectional area of the sphere. The sphere is assumed to be much smaller than any geometric details but much larger than the wavelength of the radiation, so that Mie scattering can be neglected.

This feature is available when the ray power is solved for. The variable for fluence rate is <phys>.<name>.E0, where <phys> is the name of the Geometrical Optics physics interface and <name> is the name of the physics feature, for example gop.frc1.E0.

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Q    Fluence Rate Calculation Theory

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## *Deposited Ray Power (Domain)*

The **Deposited Ray Power** node is used to compute a heat source based on the attenuation of rays as they propagate through a domain with a complex refractive index. This feature is available when the ray power is solved for. The variable for deposited power is <name>.Qsrc, where <name> is the name of the Geometrical Optics physics interface, for example gop.Qsrc.

| 🔍 | Attenuation Within Domains |
|---|---|

### *Deposited Ray Power (Boundary)*

When the ray power is solved for, the **Deposited Ray Power** subnode is available from the context menu (right-click the Wall, parent node) or from the **Physics** toolbar, **Attributes** menu. The **Deposited Ray Power** subnode computes the total incident energy flux on a surface based on the power of incident rays.

#### SMOOTHING
Select the **Compute smoothed accumulated variable** check box to enter a **Smoothing radius** $r$ (SI unit: m) The smoothing radius functions like the corresponding setting for the Accumulator (Boundary) node.

### *Accumulator (Domain)*

Use the **Accumulator** node to define additional degrees of freedom on a domain. Each **Accumulator** defines a variable, called the accumulated variable, on each domain element in the selection list. The values of the accumulated variables are determined by the properties of rays in each domain element.

#### ACCUMULATOR SETTINGS
Select an **Accumulator type**: **Density** (default) or **Count**.

- For **Density** the accumulated variable is divided by the volume of the mesh element where it is defined.

- For **Count** the accumulated variable is unaffected by the element size.

Select an option from the **Accumulate over** list: **Elements** (the default) or **Elements and time**.

- For **Elements** the value of the accumulated variable in an element is the sum of the source terms of all rays in that element. If the **Accumulator type** is set to **Density**, this sum is divided by the mesh element volume.

- For **Elements and time** the time derivative of the accumulated variable in an element is the sum of the source terms of all rays in that element. If the **Accumulator type** is

set to **Density**, this sum is divided by the mesh element volume. As each ray propagates through a series of mesh elements, it leaves behind a contribution to the accumulated variable that remains even after the ray has moved on.

Enter the **Accumulated variable name**. The default is rpd. The accumulated variable is defined as <name>.<varname>, where <name> is the physics interface name and <varname> is the accumulated variable name. For example, in an instance of the Geometrical Optics interface with default name gop and default accumulated variable name rpd, the variable would be named gop.rpd.

Enter a **Source** $R$. The unit of the source depends on the settings in the **Units** section. The source term is used to calculate the accumulated variable in a manner specified by the **Accumulate over** and **Accumulator type** settings.

If **Elements and time** is selected from the **Accumulate over** list, select an option from the **Source interpolation** list: **Constant**, **Linear** (the default), **Quadratic**, or **Exponential**. The **Source interpolation** determines what functional form the **Source** is assumed to follow during each time step taken by the solver. This information is used to compute the accumulated variable in mesh elements that the rays pass through during each time step.

### UNITS

Select a **Dependent variable quantity** from the list; the default is **Dimensionless [I]**. To enter a unit, select **None** from the list and in the **Unit** field enter a value, for example, K, m/s, or mol/m^3.

## *Accumulator (Boundary)*

The **Accumulator** subnode is available from the context menu (right-click the Wall or Material Discontinuity parent node) or from the **Physics** toolbar, **Attributes** menu. Each **Accumulator** subnode defines a variable, called the accumulated variable, on each boundary element in the selection of the parent node. The accumulated variables are incremented when rays interact with the boundaries where they are defined.

### ACCUMULATOR SETTINGS

Select an option from the **Accumulator type** list: **Density** (default) or **Count**.

- For **Density** the accumulated variable is divided by the surface area of the boundary element where it is defined.

- For **Count** the accumulated variable is the sum of the source terms of all rays that hit the boundary element, and is unaffected by the boundary element size.

Select an option from the **Accumulate over** list: **Ray-wall interactions** (the default) or **Rays in boundary elements**.

- For **Ray-wall interactions** the accumulated variable is affected by all rays that hit the boundary element.
- For **Rays in boundary elements** the accumulated variable is only affected by rays that freeze or stick to the boundary element.

Enter the **Accumulated variable name**. The default is rpb. The accumulated variable is defined as <scope>.<name>, where <scope> includes the name of the physics interface node, parent boundary condition, and the **Accumulator** node, and <name> is the accumulated variable name.

For example, if the **Accumulator** subnode is added to a Wall node in an instance of the Geometrical Optics interface using the default variable name rpb, the accumulated variable name might be gop.wall1.bacc1.rpb.

Enter a **Source** $R$. The unit of the source term depends on the settings in the **Units** section. Whenever a ray collides with a boundary element in the selection of the parent node, the accumulated variable in that element is incremented by the source term. If the **Accumulator type** is set to **Density**, the source term is divided by the area of the boundary element (in 3D) or the length of the boundary element (in 2D).

For example, if the source is 1 and **Count** is selected from the **Accumulator type** list, a variable is created to store the number of times each boundary element is hit by a ray.

### UNITS

Select a **Dependent variable quantity** from the list; the default is **Dimensionless [1]**. To enter a unit, select **None** from the list and in the **Unit** field enter a value, for example, K, m/s, or mol/m^3.

### SMOOTHING

The accumulated variables are computed using discontinuous shape functions. Select the **Compute smoothed accumulated variable** check box to compute a smoothed accumulated variable by computing the average value of the variable within a sphere of a user-defined radius. Then enter a **Smoothing radius** $r$ (SI unit: m). The default is 1 m.

Accumulator Theory: Boundaries

## Nonlocal Accumulator

Use the **Nonlocal Accumulator** subnode to communicate information from a ray's current position to the position from which it was released.

The subnode is available from the context menu (right-click the Release from Boundary parent node) or from the **Physics** toolbar, **Attributes** menu.

Each **Nonlocal accumulator** subnode defines a variable, called the accumulated variable, that is computed using variables defined on rays released by the parent **Release from Boundary** node or on domains and boundaries encountered by such rays.

### ACCUMULATOR SETTINGS

Select an **Accumulator type**: **Density** (default) or **Count**.

- For **Density** the accumulated variable is divided by the volume of the mesh element where it is defined.
- For **Count** the accumulated variable is unaffected by the element size.

Select an option from the Accumulate over list: **Elements** (default) or **Elements and time**.

- For **Elements** the accumulated variable is proportional to the instantaneous value of the **Source** term $R$ for all applicable rays.
- For **Elements and time** the time derivative of the accumulated variable is proportional to the instantaneous value of the **Source** term $R$ for all applicable rays, and thus the accumulated variable considers the time history of rays in the modeling domain instead of just their current values.

Enter the **Accumulated variable name**. The default is rpi.

Enter a **Source** $R$. The unit of the source depends on the settings in the **Units** section. The source term is used to calculate the accumulated variable in a manner specified by the **Accumulate over** and **Accumulator type** settings.

Select a **Source geometric entity level**: **Domains**, **Boundaries**, or **Domains and boundaries**.

- If **Domains** is selected, rays only contribute to the accumulated variable on their releasing surface while they are active (still propagating through a domain).
- If **Boundaries** is selected, the rays only contribute to the accumulated variable if they have become stuck or frozen to a boundary somewhere in the model.
- If **Domains and boundaries** is selected, all of the active, stuck, and frozen rays released by a feature can contribute to the accumulated variable.

Select a **Dependent variable quantity** from the list; the default is **Dimensionless [I]**. To enter a unit, select **None** from the list and in the **Unit** field enter a value.

### SMOOTHING

Select the **Compute smoothed accumulated variable** check box to enter a **Smoothing radius** $r$ (SI unit: m). The default is $0.1$ m.

## Auxiliary Dependent Variable

Use the **Auxiliary Dependent Variable** node to solve additional first-order ordinary differential equations for each ray released.

### AUXILIARY DEPENDENT VARIABLE

Enter a **Field variable name**. The default is rp and can be changed to anything provided it does not conflict with the name of the variables for the position or momentum degrees of freedom, or with other auxiliary dependent variables.

Enter a **Source** $R$. The unit of the source depends on the unit of the auxiliary dependent variable and the option selected from the **Integrate** list described below.

Select a way to **Integrate** the equation you have defined: **With respect to time** or **Along ray trajectory**. For example, to reproduce the variable for optical path length, you could set the **Source** to $1$ and set **Integrate** to **Along ray trajectory**. To compute the length of the ray trajectory you can set the **Source** to $1$ and set **Integrate** to **Along ray trajectories**.

### UNITS

These settings are the same as for Accumulator (Domain).

## Ray Continuity

Use the **Ray Continuity** node to specify that rays should cross a pair boundary as if it were invisible. Pair boundaries appear when the geometry sequence ends in **Form Assembly** instead of **Form Union**. Such boundaries require special handling because the mesh elements on either side of the pair boundary are not required to match up exactly.

### PAIR SELECTION

Select one or more identity pairs to allow rays to cross between the source and destination boundaries of these pairs. Such identity pairs are typically created

automatically on interior boundaries when the geometry sequence ends in a **Form Assembly** node instead of a **Form Union** node.

> The **Ray Continuity** node does not cause the ray position components to change discontinuously; the source and destination boundaries for the identity pairs must be overlapping.
>
> If the geometry sequence ends in a **Form Union** node, the **Ray Continuity** node usually is not needed because rays can freely cross interior boundaries where no boundary condition has been applied.

## *Ray Detector*

Use the **Ray Detector** feature to compute information about rays that are located in a set of selected domains or on a set of selected boundaries. The detector may detect all rays or only the rays released by a specified release feature. Computed variables are the number of rays transmitted, the transmission probability, and a logical expression which can be used to filter the rendered rays during results processing.

The **Ray Detector** feature is also capable of computing the total transmitted ray power. If the ray power is solved for, then a global variable for the total power transmitted to the detector is available.

### RAY DETECTOR

Select an option from the **Release feature** list: **All** (the default), or any of the features which are capable of releasing rays. When **All** is selected, the variables computed are summed over all release features in the model.

# Theory for the Geometrical Optics Interface

The Geometrical Optics Interface theory is described in this section. The following sections are listed in the order in which they appear:

- Note on Sign Conventions
- The Electromagnetic Wave Equation
- Introduction to Geometrical Optics
- Optical Dispersion Models
- Thermo-Optic Dispersion Models
- Optical Attenuation Models
- Initial Conditions: Position
- Initial Conditions: Direction
- Initial Conditions: Wavelength or Frequency
- Blackbody Radiation Theory
- Gaussian Beam Theory
- Material Discontinuity Theory
- The Fresnel Equations
- Intensity, Wavefront Curvature, and Polarization
- Wavefront Curvature Calculation in Graded Media
- Refraction in Strongly Absorbing Media
- Attenuation Within Domains
- Ray Termination Theory

- Illuminated Surface Theory
- Theory of Mueller Matrices and Optical Components
- Thin Dielectric Film Theory
- Diffraction Grating Theory
- Ideal Lens Theory
- Surface Scattering Theory
- Volumetric Scattering Theory
- Interference Pattern Theory
- Monochromatic Aberrations and the Zernike Polynomials
- Accumulator Theory: Domains
- Accumulator Theory: Boundaries
- References for the Geometrical Optics Interface

## Note on Sign Conventions

When describing the propagation of a plane electromagnetic wave, different references will employ different sign conventions. The choice of sign convention can have far-reaching implications for the interpretation of phase delays and material properties, among other things.

A plane electromagnetic wave is sometimes defined as

$$\mathbf{E} = \mathbf{E}_0 \exp[i(\mathbf{k} \cdot \mathbf{r} - \omega t)] \tag{3-1}$$

and at other times as

$$\mathbf{E} = \mathbf{E}_0 \exp[i(\omega t - \mathbf{k} \cdot \mathbf{r})] \tag{3-2}$$

where

- $\mathbf{E}$ (SI unit: V/m) is the electric field along the ray,
- $\mathbf{E}_0$ (SI unit: V/m) is the electric field amplitude at $\mathbf{r} = \mathbf{0}$ and $t = 0$,
- $\mathbf{k}$ (SI unit: rad/m) is the wave vector,
- $\mathbf{r}$ (SI unit: m) is the position vector,
- $\omega$ (SI unit: rad/s) is the angular frequency, and
- $t$ (SI unit: s) is time.

For example, Refs. 1 and 9 use the sign convention in Equation 3-1, whereas Refs. 10, 12, 15, 17, and 20 use the sign convention in Equation 3-2.

Suppose that the wave propagates in the positive $x$ direction. Then the wave vector may be defined as

$$k = \left( \frac{\omega n}{c}, 0, 0 \right)$$

where $n$ (dimensionless) is the refractive index of the medium, assumed to be isotropic. For an absorbing or gain medium, $n$ is complex-valued. Using Equation 3-1, the electric field along a plane wave in an absorbing or gain medium is

$$\mathbf{E} = \mathbf{E}_0 \exp[-i\omega t] \exp\left[ i\frac{\omega}{c} x \operatorname{Re}(n) \right] \exp\left[ -\frac{\omega}{c} x \operatorname{Im}(n) \right]$$

which has an exponentially decaying magnitude (absorbing medium) if the imaginary part of $n$ is positive, and an exponentially growing magnitude (gain medium) if the

imaginary part of $n$ is negative. In contrast, when starting from Equation 3-2, the electric field is

$$\mathbf{E} = \mathbf{E}_0 \exp[i\omega t] \exp\left[-i\frac{\omega}{c}x\mathrm{Re}(n)\right]\exp\left[\frac{\omega}{c}x\mathrm{Im}(n)\right]$$

So the medium is absorbing if the imaginary part of $n$ is negative, or a gain medium if the imaginary part of $n$ is positive.

The Geometrical Optics interface uses the convention of Equation 3-2. Therefore the complex-valued refractive index may be written as $n - i\kappa$, where both $n$ and $\kappa$ are real-valued. The variable $\kappa$, sometimes called the extinction coefficient, should then be positive when defining an absorbing medium, for example when specifying the **Refractive index, imaginary part** in the Medium Properties node.

## *The Electromagnetic Wave Equation*

The relationships between the electric and magnetic fields are together known as Maxwell's Equations (Ref. 10),

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}$$

$$\nabla \cdot \mathbf{D} = \rho$$

$$\nabla \cdot \mathbf{B} = 0$$

where

- **E** (SI unit: V/m) is the electric field,
- **D** (SI unit: $C/m^2$) is the electric displacement,
- **H** (SI unit: A/m) is the magnetic field,
- **B** (SI unit: $Wb/m^2$) is the magnetic flux density or magnetic induction,
- $\rho$ (SI unit: $C/m^3$) is the charge density, and
- **J** (SI unit: $A/m^2$) is the current density.

The above equations are formulated in SI units. In Gaussian units (Ref. 9), the equations may be presented with additional factors of $4\pi$ and some additional divisions by the speed of light in a vacuum $c$.

The electric and magnetic quantities are further governed by the constitutive relations

$$\mathbf{D} = \varepsilon\mathbf{E}$$
$$\mathbf{B} = \mu\mathbf{H}$$

where $\varepsilon$ (SI unit: F/m) is the electric permittivity and $\mu$ (SI unit: H/m) is the magnetic permeability. Generally $\varepsilon$ and $\mu$ are tensors of rank 2 but they can be treated as scalar quantities if the medium is isotropic.

In a medium that is charge-free, current-free, homogeneous, and isotropic, the first two of Maxwell's Equations may be simplified to

$$\nabla \times \mathbf{E} = -\mu\frac{\partial\mathbf{H}}{\partial t}$$
$$\nabla \times \mathbf{H} = \varepsilon\frac{\partial\mathbf{E}}{\partial t}$$

One of the two remaining field variables can be eliminated by substitution, giving the so-called "curl-curl" equation for the remaining field,

$$\nabla \times \frac{1}{\mu}\nabla \times \mathbf{E} + \varepsilon\frac{\partial^2\mathbf{E}}{\partial t^2} = 0$$
$$\nabla \times \frac{1}{\varepsilon}\nabla \times \mathbf{H} + \mu\frac{\partial^2\mathbf{H}}{\partial t^2} = 0$$

If the medium is homogeneous, meaning it has spatially independent dielectric properties, then the factors of $\varepsilon$ and $\mu$ can be taken outside the curl operator, and then using the identity

$$\nabla \times \nabla \times \mathbf{E} = \nabla(\nabla \cdot \mathbf{E}) - \nabla^2\mathbf{E}$$

and recalling that the fields are divergence-free, the electromagnetic wave equation may be written as

$$\nabla^2\mathbf{E} - \mu\varepsilon\frac{\partial^2\mathbf{E}}{\partial t^2} = 0$$
$$\nabla^2\mathbf{H} - \mu\varepsilon\frac{\partial^2\mathbf{H}}{\partial t^2} = 0$$

Thus, either the electric field or magnetic field can be obtained by solving a vector Helmholtz equation. Here the electric field will be used.

The vector Helmholtz equation permits a variety of different solutions, one of which is a plane electromagnetic wave,

$$\mathbf{E} = \mathbf{E}_0\cos(\omega t - \mathbf{k} \cdot \mathbf{r})$$

where

- $\mathbf{k}$ (SI unit: rad/m) is the wave vector,
- $\mathbf{r}$ (SI unit: m) is the position vector,
- $\omega$ (SI unit: rad/s) is the angular frequency,
- $t$ (SI unit: s) is time, and
- $\mathbf{E}_0$ (SI unit: V/m) is the complex-valued electric field amplitude at $\mathbf{r} = \mathbf{0}$ and $t = 0$.

It is more common to express $\mathbf{E}$ as the exponential of a complex phase,

$$\mathbf{E} = \mathbf{E}_0 \exp[i(\omega t - \mathbf{k} \cdot \mathbf{r})]$$

Although the real operator is not explicitly applied here, it should be understood that only the real part of this expression for $\mathbf{E}$ has any physical significance, and that the imaginary part is just a mathematical construction.

The form of the electric field is a set of plane surfaces of constant phase that propagate forward at the phase velocity

$$v_p = \frac{\omega}{k} \tag{3-3}$$

Where $k$ is the magnitude of the wave vector $\mathbf{k}$. This is the speed of light in the medium.

Differentiating $\mathbf{E}$ gives

$$\frac{\partial \mathbf{E}}{\partial t} = i\omega \mathbf{E}$$

$$\nabla \cdot \mathbf{E} = -i(\mathbf{k} \cdot \mathbf{E})$$

However, since $\mathbf{E}$ is divergence-free, $\mathbf{k}$ and $\mathbf{E}$ must be orthogonal. The same can be deduced about $\mathbf{k}$ and $\mathbf{H}$. In addition, from Maxwell's Equations,

$$\nabla \times \mathbf{H} = i\omega\varepsilon \mathbf{E}$$

So that $\mathbf{k}$, $\mathbf{E}$, and $\mathbf{H}$ are all orthogonal.

Substituting the electromagnetic plane wave definition back into the electromagnetic wave equation yields

$$k^2 \mathbf{E} - \mu\varepsilon\omega^2 \mathbf{E} = 0$$

So the relationship between the angular frequency and wave vector norm is

$$k = \omega\sqrt{\mu\varepsilon} \qquad\qquad (3\text{-}4)$$

Comparing Equation 3-3 and Equation 3-4 shows that

$$v_p = \frac{1}{\sqrt{\mu\varepsilon}}$$

Now express the permittivity and permeability as

$$\varepsilon = \varepsilon_r\varepsilon_0 \qquad \mu = \mu_r\mu_0$$

where

- $\varepsilon_0$ = 8.854187817 $\times$ 10$^{-12}$ F/m is the vacuum permittivity,
- $\mu_0$ = 1.256637062 $\times$ 10$^{-6}$ H/m is the vacuum permeability,
- $\varepsilon_r$ (dimensionless) is the relative permittivity of the medium, and
- $\mu_r$ (dimensionless) is the relative permeability of the medium.

Noting that

$$c = \frac{1}{\sqrt{\mu_0\varepsilon_0}}$$

where c = 2.99792458 $\times$ 10$^8$ m/s is the speed of light in a vacuum, the phase velocity is

$$v_p = \frac{c}{\sqrt{\mu_r\varepsilon_r}}$$

At optical frequencies, many materials are nonmagnetic, $\mu_r$ = 1. In that case, the phase velocity is just $c/n$, where

$$n = \sqrt{\varepsilon_r}$$

is the refractive index of the material. Thus, for linear nonmagnetic materials,

$$k = \frac{\omega}{c}n$$

If the medium absorbs energy from the propagating wave or adds energy to it, then the refractive index becomes a complex-valued quantity, denoted $n - i\kappa$, where $\kappa$ is called the extinction coefficient. For absorbing media, $\kappa > 0$, whereas for gain media, $\kappa < 0$.

## Introduction to Geometrical Optics

The previous sections show that Maxwell's Equations allow a plane wave solution,

$$\mathbf{E} = \mathbf{E}_0 e^{i\Psi}$$

where $\mathbf{E}_0$ is the slowly varying amplitude and the phase $\Psi$ is a function of the position vector $\mathbf{q}$ and time $t$. If the field is observed only at locations that are very far from any source, the phase can be expressed as

$$\Psi = \omega t - \mathbf{k} \cdot \mathbf{q} + \alpha$$

where $\mathbf{k}$ is the wave vector, $\omega$ is the angular frequency, and $\alpha$ is an arbitrary phase shift. In an isotropic medium, the wave vector and the angular frequency are further related by the expression

$$\omega = \frac{c|\mathbf{k}|}{n(\mathbf{q})}$$

where $n(\mathbf{q})$ is the refractive index of the medium. It follows that the wave vector and angular frequency can be expressed in terms of the phase:

$$\mathbf{k} = \frac{\partial \Psi}{\partial \mathbf{q}} \qquad \omega = -\frac{\partial \Psi}{\partial t}$$

Following Landau and Lifshitz in Ref. 1, the wave vector and frequency are analogous to the generalized momentum $\mathbf{p}$ and Hamiltonian $H$ of a solid particle,

$$\mathbf{p} = \frac{\partial S}{\partial \mathbf{q}} \qquad H = -\frac{\partial S}{\partial t}$$

where $S$ is the integral of the Lagrangian along the particle's trajectory. From this analogy, it follows that the ray trajectory can be computed by solving six coupled first-order ordinary differential equations for the components of $\mathbf{k}$ and $\mathbf{q}$:

$$\frac{d\mathbf{k}}{dt} = -\frac{\partial \omega}{\partial \mathbf{q}} \qquad \frac{d\mathbf{q}}{dt} = \frac{\partial \omega}{\partial \mathbf{k}}$$

In regions of constant refractive index, the simplified equations of motion are:

$$\frac{d\mathbf{k}}{dt} = 0 \qquad \frac{d\mathbf{q}}{dt} = \frac{c\mathbf{k}}{n|\mathbf{k}|}$$

These first-order equations for the ray trajectory are only valid in regions that are many wavelengths away from any point source; that is, $\Psi \gg 1$.

## Optical Dispersion Models

The **Refractive index, real part**, $n$ (dimensionless) may be expressed as a function of wavelength using an optical dispersion model. The **Optical dispersion model** for domains outside the selection can be specified in the **Geometrical Optics** interface. Domains that are included in the Geometrical Optics interface selection have dispersion models that are specified in the **Medium Properties** feature.

### THE REFRACTIVE INDEX OF AIR

A dispersion model for the refractive index of air can be used in exterior and unmeshed domains. It can also be used to convert from relative to absolute refractive indices (see below). The Edlén (1953) air model, described in Ref. 2, which gives the refractive index of air $n_{air}$ as a function of wavelength, temperature, and pressure is

$$n_{air}(\lambda_0, T, P) = 1 + \frac{n_{air, STP}(\lambda_0) - 1}{1 + 3.4785 \times 10^{-3}(T - T_{std})} \frac{P}{P_{std}} \qquad (3\text{-}5)$$

where $T$ is the temperature (SI unit: K) and $P$ is the pressure (SI unit: Pa). The refractive index of air at standard temperature and pressure, $n_{air,STP}$, is given by

$$n_{air, STP}(\lambda_0) = 1 + 10^{-8} \times \left( 6432.8 + \frac{2,949,810\lambda'^2}{146\lambda'^2 - 1} + \frac{25,540\lambda'^2}{41\lambda'^2 - 1} \right)$$

where, by definition, the standard temperature is $T_{std} = 15°C$ and the standard pressure is $P_{std} = 101,325$ Pa (and with a $CO_2$ concentration of 0.03%) with the wavelength given in microns; that is $\lambda' = \lambda/1[\mu m]$.

### RELATIVE VS. ABSOLUTE REFRACTIVE INDICES

It is important to appreciate that the refractive indices given by manufacturers are often relative to air at a certain temperature and pressure. Therefore, each of the optical dispersion models (except **Temperature-dependent Sellmeier**) require a reference temperature $T_{ref}$ (SI unit: K) and pressure $P_{ref}$ (SI unit: Pa) to be specified. This is interpreted to be the temperature and pressure of the air in which the refractive indices used to generate the model were measured. The reference pressure is absolute. If the reference pressure $P_{ref} \neq 0$, then it is assumed that the dispersion model will give relative refractive indices $n_{rel}$ (dimensionless). The conversion of refractive index from relative ($n_{rel}$) to absolute ($n$) is made using a model for the refractive index of air ($n_{air}$). That is,

$$n = n_{rel} \times n_{air}$$

with $n_{air}$ defined in Equation 3-5 with $T = T_{ref}$ and $P = P_{ref}$.

**AVAILABLE OPTICAL DISPERSION MODELS**

Each model requires a set of coefficients to be specified. These can be determined, for example, by making a least squares fit to a set of refractive index measurements at discrete wavelengths. At least one optical dispersion model (**Temperature-dependent Sellmeier**) allows the refractive index to be expressed as a function of both wavelength and temperature. All other optical dispersion models may be used together with a thermo-optic dispersion model to calculate a temperature-dependent shift in the refractive index. This is discussed in Thermo-Optic Dispersion Models.

The built-in optical dispersion models are listed in Table 3-3.

TABLE 3-3: LIST OF OPTICAL DISPERSION MODELS

| NAME | EXPRESSION |
|------|------------|
| Cauchy | $n_{rel} = A + \dfrac{B}{\lambda^2} + \dfrac{C}{\lambda^4}$ |
| Conrady | $n_{rel} = A + \dfrac{B}{\lambda} + \dfrac{C}{\lambda^{3.5}}$ |
| Herzberger | $n_{rel} = A_0 + \dfrac{A_1}{\lambda^2 - 0.028} + \dfrac{A_2}{(\lambda^2 - 0.028)^2} + A_3\lambda^2 + A_4\lambda^4$ |
| Schott | $n_{rel}^2 = A_0 + A_1\lambda^2 + \dfrac{A_2}{\lambda^2} + \dfrac{A_3}{\lambda^4} + \dfrac{A_4}{\lambda^6} + \dfrac{A_5}{\lambda^8}$ |
| Schott extended | $n_{rel}^2 = A_0 + A_1\lambda^2 + A_2\lambda^4 + \dfrac{A_3}{\lambda^2} + \dfrac{A_4}{\lambda^4} + \dfrac{A_5}{\lambda^6} + \dfrac{A_6}{\lambda^8} + \dfrac{A_7}{\lambda^{10}} + \dfrac{A_8}{\lambda^{12}}$ |
| Sellmeier | $n_{rel}^2 = 1 + \dfrac{A_1\lambda^2}{\lambda^2 - B_1} + \dfrac{A_2\lambda^2}{\lambda^2 - B_2} + \dfrac{A_3\lambda^2}{\lambda^2 - B_3}$ |
| Sellmeier modified, type I | $\dfrac{n_{rel}^2 - 1}{n_{rel}^2 + 2} = \dfrac{A_1\lambda^2}{\lambda^2 - B_1} + \dfrac{A_2\lambda^2}{\lambda^2 - B_2} + \dfrac{A_3\lambda^2}{\lambda^2 - B_3}$ |

TABLE 3-3: LIST OF OPTICAL DISPERSION MODELS

| NAME | EXPRESSION |
|---|---|
| Sellmeier modified, type 2 | $n_{\text{rel}}^2 = A + \dfrac{B_1 \lambda^2}{\lambda^2 - C_1} + \dfrac{B_2 \lambda^2}{\lambda^2 - C_2}$ |
| Temperature - dependent Sellmeier | $n^2 = 1 + \displaystyle\sum_{i=1}^{3} \dfrac{S_i(T)\lambda^2}{\lambda^2 - \lambda_i^2(T)}, \ S_i(T) = \displaystyle\sum_{j=0}^{4} S_{ij}T^j, \lambda_i(T) = \displaystyle\sum_{j=0}^{4} \lambda_{ij}T^j$ |

All optical dispersion models assume that coefficients have been determined with expressions where the wavelengths have units of μm. For example, in the Schott model, the coefficients have units $1$, μm, $\mu m^2$, $\mu m^3$, and so on. The input wavelength can still have any unit; the normalization to microns is done automatically.

The **Temperature-dependent Sellmeier** model (Ref. 3, Ref. 4) assumes coefficients based on absolute temperature specified in Kelvin (K).

## Thermo-Optic Dispersion Models

The **Refractive index, real part**, $n$ (dimensionless) may be expressed as a function of both wavelength and temperature by using an expression of the form

$$n(\lambda, T) = n(\lambda) + \Delta n(\lambda, T).$$

The wavelength-dependent (non-temperature-dependent) component of this equation, $n(\lambda)$, might be any one of the optical dispersion models discussed above, or it could be specified by other means. The change in refractive index as a function of temperature, $\Delta n(\lambda, T)$ can be computed using a thermo-optic dispersion model.

### SCHOTT THERMO-OPTIC DISPERSION MODEL

An expression for the change in refractive index as a function of temperature, $\Delta n(\lambda, T)$ is given in Ref. 5. It may be derived by integrating the dispersion formula for the thermo-optic coefficient $(dn/dT)$. That is,

$$\frac{dn(\lambda, T)}{dT} = \frac{n^2(\lambda, T_0) - 1}{2n(\lambda, T_0)} \left( D_0 + 2D_1 \Delta T + 3D_2 \Delta T^2 + \frac{E_0 + 2E_1 \Delta T}{\lambda^2 - \lambda_{\text{TK}}^2} \right),$$

which gives

$$\Delta n(\lambda,T) \;=\; \frac{n(\lambda,T_0)-1}{2n(\lambda,T_0)}\left(D_0\Delta T + D_1\Delta T^2 + D_2\Delta T^3 + \frac{E_0\Delta T + E_1\Delta T^2}{\lambda^2 - \lambda_{TK}^2}\right).$$

In the above formula $T_0$ is the reference temperature against which the temperature difference $\Delta T = T - T_0$ is computed and $D_0, D_1, D_2, E_0, E_1$, and $\lambda_{TK}$, are glass-specific coefficients.

### Refractive Index at Common Spectral Lines

Predefined postprocessing variables are available for the refractive index at frequently used spectral lines (Ref. 6):

- $n_d$ is the d-line refractive index (yellow helium spectral line, 587.56 µm)

- $n_F$ is the F-line refractive index (blue hydrogen spectral line, 486.13 µm)

- $n_C$ is the C-line refractive index (red hydrogen spectral line, 656.28 µm)

In addition, the dimensionless Abbe number $V_d$ is automatically defined,

$$V_d \;=\; \frac{n_d - 1}{n_F - n_C}$$

The Abbe number indicates the sensitivity of the glass refractive index to changes in wavelength across the visible part of the electromagnetic spectrum. A greater Abbe number means that a singlet lens of the material would exhibit less chromatic aberration, while a singlet lens of a lower Abbe number would be more susceptible to chromatic aberration.

> For more instructions on postprocessing of the refractive index in Geometrical Optics models, see Plotting Refractive Index and Abbe Number in the Ray Optics Modeling chapter.

### Optical Attenuation Models

Most real-world media absorb some energy from the electromagnetic waves that pass through them, converting this energy into another form such as heat. A medium might also redirect some energy without absorbing it, a phenomenon called scattering which will be explored in a later section.

In the Geometrical Optics interface, an absorbing medium has a complex-valued refractive index of the form $n - i\kappa$., where $n$ and $\kappa$ are real numbers and $\kappa > 0$. As a ray propagates through an absorbing medium, the built-in variables that track ray intensity and power may decrease.

> There is yet another phenomenon that influences the calculation of the built-in variable for ray intensity: the convergence or divergence of the wavefront. For simplicity this is not considered here (the rays are assumed to represent plane waves) but will be revisited in a later section.

Recall that the electric field amplitude of a plane electromagnetic wave in a medium of complex-valued refractive index $n - i\kappa$ is

$$\mathbf{E} = \mathbf{E}_0 \exp[i\omega t] \exp\left[-i\frac{\omega}{c} x \mathrm{Re}(n)\right] \exp\left[\frac{\omega}{c} x \mathrm{Im}(n)\right]$$

Noting that the intensity is proportional to $\mathbf{E} \cdot \mathbf{E}^\star$, the imaginary terms in the exponents vanish, leaving only the attenuation term,

$$I = I_0 \exp\left[2\frac{\omega}{c} x \mathrm{Im}(n)\right] = I_0 \exp\left[-2\frac{\omega}{c}\kappa x\right]$$

Then, using the relationship

$$\frac{\omega}{c} = k_0 = \frac{2\pi}{\lambda_0}$$

the intensity decays exponentially according to

$$I = I_0 \exp\left[-\frac{4\pi\kappa}{\lambda_0} x\right]$$

In the physics interface Medium Properties node, you can control how the value of $\kappa$ is defined by selecting different options from the **Optical attenuation model** list.

### EXTINCTION COEFFICIENT
For **Extinction coefficient**, enter the value of $\kappa$ directly.

### ATTENUATION COEFFICIENT
For **Attenuation coefficient**, enter the value or expression of the coefficient $\alpha$, defined as

$$\alpha \equiv \frac{4\pi\kappa}{\lambda_0}$$

Thus

$$I = I_0 \exp[-\alpha x]$$

## INTERNAL TRANSMITTANCE

The **Optical attenuation model** list also includes the following options:

- **Internal transmittance, 2 mm sample thickness**

- **Internal transmittance, 5 mm sample thickness**

- **Internal transmittance, 10 mm sample thickness**

- **Internal transmittance, 25 mm sample thickness**

The internal transmittance is the fraction of the ray intensity that is transmitted, rather than absorbed, through a sample of the given thickness $d$, neglecting Fresnel losses at the surfaces of the sample. Setting $x = d$ in the previous equations,

$$\tau_{i,d} \equiv \frac{I}{I_0} = \exp\left[-\frac{4\pi\kappa}{\lambda_0}d\right]$$

Solving this equation for $\kappa$ yields

$$\kappa = -\frac{\lambda_0}{4\pi d}\log\tau_{i,d} \tag{3-6}$$

This result is positive or zero because the internal transmittance cannot exceed unity.

*Internal Transmittance Data and Numerical Precision*

If internal transmittance data is tabulated for different glasses and different wavelengths, and all internal transmittance values are reported to the same number of digits, loss of precision may occur if the internal transmittance data for a very thin sample of a weakly absorbing glass, or a thick sample of a very strongly absorbing glass, is used.

To see this more concretely, suppose that internal transmittance data is available for 10 mm and 25 mm samples of a glass at $\lambda_0 = 600$ nm, each reported to three digits. Suppose the reported values are $\tau_{i,10} = 0.998$ and $\tau_{i,25} = 0.995$. Because of roundoff, we may presume the actual value of $\tau_{i,10}$ to be between 0.9975 and 0.9985, and

similarly for $\tau_{i,25}$ to be between 0.9945 and 0.9955. Substituting these lower and upper bounds into Equation 3-6 then gives the following results:

- For the 10 mm sample, $7.2 \times 10^{-9} < \kappa < 12.0 \times 10^{-9}$
- For the 25 mm sample, $8.6 \times 10^{-9} < \kappa < 10.5 \times 10^{-9}$

Therefore it would be preferable to use the data for the thicker sample if it is available.

Conversely, if the reported transmittance values were very close to zero (perhaps in the IR or UV range) it would be beneficial to use data for the thinnest sample available.

If a material uses internal transmittance data and one of the options **Extinction coefficient** or **Attenuation coefficient** is selected, the transmittance data will automatically be converted to this coefficient. If two or more sets of transmittance data for different sample thicknesses are defined for the material, the default behavior is to use the data for the thicker sample unless otherwise specified.

## *Initial Conditions: Position*

The ray release positions may be mesh based, from a user-specified grid, uniformly distributed, loaded from a file, or based on an analytic expression.

### LOADING INITIAL COORDINATES FROM FILE

If the initial ray positions are loaded from a text file using the Release from Data File node, the initial positions may be scaled, rotated, translated, or some combination of these. Assuming $\mathbf{q}_0$ to be the loaded ray release position, $\mathbf{q}_0$ can be rotated using the rotation matrix $\mathbf{A}$

$$\mathbf{q}_0' = \mathbf{A}\mathbf{q}_0$$

where $\mathbf{A}$ in 3D is given by

$$\mathbf{A} = \begin{bmatrix} \cos\alpha\cos\gamma - \sin\alpha\cos\beta\sin\gamma & -\cos\alpha\sin\gamma - \sin\alpha\cos\beta\cos\gamma & \sin\alpha\sin\beta \\ \sin\alpha\cos\gamma + \cos\alpha\cos\beta\sin\gamma & -\sin\alpha\sin\gamma + \cos\alpha\cos\beta\cos\gamma & -\cos\alpha\sin\beta \\ \sin\beta\sin\gamma & \sin\beta\cos\gamma & \cos\beta \end{bmatrix}$$

and in 2D by

$$\mathbf{A} = \begin{bmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{bmatrix}$$

In 3D, $\alpha$, $\beta$, and $\gamma$ are the Euler angles:

- First $\alpha$ rotates the position about the space-fixed $z$-axis.

- Then $\beta$ rotates the position about the $x'$-axis, that is, the body-fixed $X$-axis after rotation about the $z$-axis.

- Finally $\gamma$ rotates the position about the $z''$-axis, that is, the body-fixed $Z$-axis after rotation about the $z$-axis and $x'$-axis.

In 2D, $\alpha$ is the angle of counterclockwise rotation about the origin.

All components of the ray release position vector are multiplied by the **Scale factor**,

$$\mathbf{q}_0'' = R\mathbf{q}_0'$$

Finally, the initial positions may be translated by a displacement vector $\Delta\mathbf{q}$,

$$\mathbf{q}_0''' = \mathbf{q}_0'' + \Delta\mathbf{q}$$

The primes indicate that translation is applied after any rotation or dilation (scaling). However, because the dilation applies equally to all vector components, the dilation and rotation commute with each other, so their relative order does not matter.

## Initial Conditions: Direction

There are several options available for specifying the initial direction of rays. These options work by assigning values to the degrees of freedom corresponding to the wave vector $\mathbf{k}$ (SI unit: rad/m) of each ray.

### EXPRESSION

The default is to enter an expression for the **Ray direction vector** $\mathbf{L}_0$ (dimensionless). This vector need not have a magnitude of unity because it is always normalized automatically. The initial wave vector is

$$\mathbf{k} = \frac{\omega n \mathbf{L}_0}{c|\mathbf{L}_0|}$$

where $\omega$ (SI unit: rad/s) is the angular frequency, $c = 299{,}792{,}458$ m/s is the speed of light in a vacuum, and $n$ (dimensionless) is the refractive index.

### LOADING INITIAL DIRECTION FROM FILE

If the initial ray positions are loaded from a text file, then optionally the initial ray direction can also be loaded from the same file. If the direction is loaded from the file

and a rotation has been applied to the ray release positions, then optionally the same rotation can be applied to the initial direction.

### SPHERICAL

When **Spherical** is selected the initial wave vectors are sampled from a distribution in wave vector space at each release point. The number of rays released from each point is usually equal to the specified value $N_w$ (dimensionless), although it may be larger if the initial values of any auxiliary dependent variables are also sampled from a distribution.

In 2D the initial wave vector components are

$$k_x = \frac{\omega n}{c} \cos \theta$$

$$k_y = \frac{\omega n}{c} \sin \theta$$

where $\theta$ goes from 0 to $2\pi$ in $N_w$ steps. In 3D the initial wave vector components are sampled according to the expressions

$$k_x = \frac{\omega n}{c} \sin \theta \cos \varphi$$

$$k_y = \frac{\omega n}{c} \sin \theta \sin \varphi$$

$$k_z = \frac{\omega n}{c} \cos \theta$$

The azimuthal angle $\varphi$ is uniformly distributed from 0 to $2\pi$. The polar angle $\theta$ is sampled from the interval $[0, \pi]$ with probability density proportional to $\sin \theta$. The polar angle is arbitrarily chosen as the angle that the initial wave vector makes with the positive $z$-axis, but any direction could be chosen because the sphere is isotropic. Therefore each ray subtends approximately the same solid angle in wave vector space.

### HEMISPHERICAL

The **Hemispherical** option is the same as the **Spherical** option, except that in 2D $\theta$ goes from 0 to $\pi$ and in 3D $\theta$ goes from 0 to $\pi/2$. The angle is measured from the direction given by the **Hemisphere axis** setting.

### CONICAL

The **Conical** option is the same as the **Spherical** option, except that $\theta$ goes from 0 to $\alpha$. The angle is measured from the direction given by the **Cone axis** setting.

The **Lambertian** option releases rays within a hemisphere in 3D, but the probability distribution function is different from that of the **Hemispherical** option. Recall that for an isotropic hemispherical distribution the polar angle $\theta$ has a probability density proportional to $\sin \theta$; for the Lambertian distribution the probability density is instead proportional to $\sin \theta \cos \theta$. Because of this extra cosine term, distributions following this probability density are said to follow Lambert's cosine law.

## *Initial Conditions: Wavelength or Frequency*

As indicated in the sections Optical Dispersion Models and Thermo-Optic Dispersion Models, the refractive index of real materials is often a function of the vacuum wavelength or frequency of the propagating rays.

In the Geometrical Optics interface, you can make the released rays monochromatic or polychromatic. If the released rays are polychromatic, you can either specify their frequency $\nu$ (SI unit: Hz) or their vacuum wavelength $\lambda_0$ (SI unit: m). If the medium is not a vacuum, the actual wavelength of the rays in the medium $\lambda$ is automatically computed by dividing the vacuum wavelength by the absolute refractive index.

To trace polychromatic light, in the settings for the Geometrical Optics interface, locate the **Ray Release and Propagation** section. From the **Wavelength distribution of released rays** list, select either **Polychromatic, specify vacuum wavelength** or **Polychromatic, specify frequency**; the default is **Monochromatic**.

Then, when releasing rays into the model (for example, with a Release or Release from Grid node), you can enter a value or expression for the wavelength or frequency directly, or sample multiple values from a distribution, by selecting an option from the **Distribution Function** list in the **Vacuum Wavelength** or **Initial Ray Frequency** section.

> ⚠️ In ray release features, different options that control the number of released rays or the number of values in a distribution are multiplicative, not additive. For example, if you use the **Release** node and set the **Number of rays per release** equal to 100, then release a **Normal** distribution of frequency values and set the **Number of values** to 1000, the total number of released rays will be 100,000.

### NORMAL DISTRIBUTION
The wavelength or frequency is sampled from the distribution function

$$f(\lambda_0) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{(\lambda_0 - \mu)^2}{2\sigma^2}\right] \qquad f(\nu) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left[-\frac{(\nu - \mu)^2}{2\sigma^2}\right]$$

where $\mu$ is the mean and $\sigma$ is the standard deviation.

### LOGNORMAL DISTRIBUTION

The wavelength or frequency is sampled from the distribution function

$$f(\lambda_0) = \frac{1}{\lambda_0 \log \text{GSD} \sqrt{2\pi}}\exp\left[-\frac{(\log\lambda_0 - \log M)^2}{2\log^2 \text{GSD}}\right]$$

$$f(\nu) = \frac{1}{\lambda_0 \log \text{GSD} \sqrt{2\pi}}\exp\left[-\frac{(\log\nu - \log M)^2}{2\log^2 \text{GSD}}\right]$$

where $M$ is the median and GSD is the geometric standard deviation, which are related to the arithmetic mean $\mu$ and the standard deviation $\sigma$ by the relations

$$\mu = M\exp\left(\frac{1}{2}\log^2 \text{GSD}\right) \qquad \sigma = \mu\sqrt{\exp(\log^2 \text{GSD}) - 1}$$

### UNIFORM

The vacuum wavelength or frequency has a uniform probability within an interval bounded by the specified maximum and minimum values, and zero probability outside this interval.

### BLACKBODY

This subsection refers to the **Blackbody** option in the **Initial Ray Frequency** or **Vacuum Wavelength** section of most general-purpose ray release features such as Release and Release from Grid. These settings only affect the distribution of the spectral variable and do not affect, for example, the initial ray intensity or power. The dedicated Blackbody Radiation node also controls the ray direction distribution and the total emitted power; for more information, see Blackbody Radiation Theory.

The **Blackbody** option samples the vacuum wavelength and frequency of released rays as if they were released from a blackbody radiation source at a specified temperature; that is, the probability distribution of wavelength or frequency follows Planck's law.

To be able to speak of both wavelength and frequency at the same time, first define the dimensionless variable $x$ (not to be confused with the spatial $x$-coordinate)

$$x = \frac{h\nu}{k_B T} = \frac{hc}{k_B \lambda_0 T}$$

- $h = 6.62607015 \times 10^{-34}$ J·s is Planck's constant,
- $c = 299{,}792{,}458$ m/s is the speed of light in a vacuum,
- $k_B = 1.380649 \times 10^{-23}$ J/K is the Boltzmann constant,
- $T$ (SI unit: K) is the surface temperature,
- $\nu$ (SI unit: Hz) is the ray frequency, and
- $\lambda_0$ (SI unit: m) is the vacuum wavelength.

Then the dimensionless form of Planck's law states that the normalized probability distribution of this variable is

$$f(x) = \frac{15}{\pi^4} \frac{x^3}{e^x - 1}$$

It might be useful to exclude outliers corresponding to extremely large or small values of the wavelength or frequency when sampling from this distribution function. You can choose to specify maximum and minimum values of the wavelength or frequency, which are first converted to upper and lower limits on $x$; or you may choose to **Specify fraction of total emissive power** and then specify a fraction slightly less than 1, so that the lower and upper tails of the distribution are automatically excluded.

## Blackbody Radiation Theory

The Blackbody Radiation node releases rays diffusely from a surface (following Lambert's cosine law) with a wavelength or frequency distribution following Planck's law (if release of polychromatic rays has been enabled) and a total source power based on the Stefan-Boltzmann law (if ray power is solved for).

### IDEAL BLACKBODY RADIATION SOURCE

An ideal blackbody (Ref. 7) is an object that absorbs all radiation that is incident upon it, regardless of the body's temperature or the wavelength of the radiation.

Consider a blackbody and some other object (not a blackbody) of the same size and shape, at the same temperature. Because, by definition, the blackbody absorbs more radiation than the other object, it must also emit more radiation than the other object

in order to maintain thermal equilibrium. Therefore an ideal blackbody is both the most efficient absorber and emitter of radiation.

### SPECTRAL EMISSIVITY AND GRAYBODY RADIATION

Real-world objects usually do not behave as ideal blackbody radiation sources. The spectral emissivity $\varepsilon(\lambda, T)$ of an object (dimensionless) is the radiant energy flux per unit surface area the object releases, divided by the radiant energy flux per unit surface area that an ideal blackbody at the same temperature would release. By definition, $\varepsilon = 1$ for an ideal blackbody.

A graybody is a radiation-emitting body whose emissivity is a constant, independent of temperature and wavelength, but not necessarily equal to 1. Blackbody radiation is thus a special case of graybody radiation, which itself is a special case out of all possible spectral emissivity functions.

### RADIOMETRIC VS ACTINOMETRIC QUANTITIES

The amount of radiation released by an object may be quantified in different ways. In the COMSOL implementation, radiometric quantities are used, meaning that the radiation is described by the amount of energy it transmits. Typical units include watts, watts per square meter, watts per square meter per steradian, watts per square meter per unit wavelength, and so on.

An alternative way to describe the amount of radiation is by using actinometric quantities, which describe the number of photons released rather than the amount of energy. From quantum mechanics, the energy of one photon, the quantum of the electromagnetic field, is defined as $E = h\nu$, where $\nu$ is the frequency (SI unit: Hz) and $h = 6.62607015 \times 10^{-34}$ J·s is Planck's constant. Currently the Geometrical Optics interface does not automatically define any variables in actinometric units.

### EXITANCE AND SPECTRAL EXITANCE

The total radiant exitance $M_e^b$ (SI unit: W/m$^2$) is the amount of electromagnetic energy emitted from the surface of the blackbody radiation source per unit time, per unit surface area.

The energy released from a blackbody source follows a wavelength distribution. For some value of the wavelength $\lambda$, imagine a sensor that detects 100% of the radiation having wavelengths between $\lambda$ and $\lambda + d\lambda$, where $d\lambda$ is an infinitesimally small change in the wavelength, but detects 0% of radiation outside this range. Then the amount of energy detected by this sensor is $M_{e,\lambda}^b d\lambda$, where $M_{e,\lambda}^b$ is the spectral radiant exitance.

The units of spectral radiant exitance are energy per unit time per unit surface area, per unit wavelength.

The most concise way to write the unit is $W/m^3$ but sometimes it is more conveniently expressed with the area and wavelength units written separately, for example, $W/(cm^2 \cdot \mu m)$. The spectral radiant exitance is usually a function of wavelength and temperature, so it may be written as $M_{e,\lambda}^b(\lambda, T)$.

For any two wavelengths $\lambda_1$ and $\lambda_2$ (assume $\lambda_1 < \lambda_2$), the total energy of emitted radiation between these wavelengths is

$$\int_{\lambda_1}^{\lambda_2} M_{e,\lambda}^b(\lambda, T)\mathrm{d}\lambda$$

The total energy released over all wavelengths is, by definition, the total radiant exitance,

$$M_e^b = \int_0^\infty M_{e,\lambda}^b(\lambda, T)\mathrm{d}\lambda$$

The spectral radiant exitance may also be written in terms of a spectral quantity other than wavelength, so long as that other quantity has a one-to-one relationship with wavelength. Other quantities that have been used include the frequency, the logarithm of frequency or wavelength, and other powers of frequency or wavelength. In fact there are infinitely many choices for the arbitrarily high powers of $\lambda$ and $\nu$, of which the first power of wavelength is historically the most common choice (Ref. 7).

The spectral radiance in terms of frequency is written $M_{e,\nu}^b(\nu, T)$ (SI unit: $W \cdot s/m^2$),

$$M_e^b = \int_0^\infty M_{e,\nu}^b(\nu, T)\mathrm{d}\nu$$

The total energy between two wavelengths $\lambda_1$ and $\lambda_2$ should be the same when converting these wavelengths to frequencies $\nu_1 = c/\lambda_1$ and $\nu_2 = c/\lambda_2$,

$$\int_{\lambda_1}^{\lambda_2} M_{e,\lambda}^b(\lambda, T)\mathrm{d}\lambda = \int_{\nu_2}^{\nu_1} M_{e,\nu}^b(\nu, T)\mathrm{d}\nu \qquad (3\text{-}7)$$

The order of the limits of integration is reversed because if $\lambda_1 < \lambda_2$, then $\nu_1 > \nu_2$.

### SPECTRAL RADIANCE

The radiance of a blackbody is the amount of energy per unit time that is released from the surface of the body and passes through a certain solid angle in the half-space adjacent to the body, per unit time, per unit solid angle, per unit projected surface area of the radiation source,

$$L_{e,\lambda}^{b}(\lambda, T) \;=\; \frac{1}{\cos\theta}\frac{d(M_{e,\lambda}^{b}(\lambda, T))}{d\Omega} \tag{3-8}$$

The term $\cos\theta$ appears in the denominator because the radiance is measured per unit projected surface area from the point of view of an observer at polar angle $\theta$, rather than the actual surface area from which the radiation is emitted.

The spectral radiance in terms of wavelength $L_{e,\lambda}^{b}(\lambda, T)$ has SI units of $W/(m^3 \cdot sr)$, or it may be written with the area units and wavelength units separated, for example $W/(cm^2 \cdot nm \cdot sr)$. Similarly the spectral radiance in terms of frequency $L_{e,\nu}^{b}(\nu, T)$ has SI units of $(W \cdot s)/(m^2 \cdot sr)$ but can also be written using different area units.

In general, the spectral radiance may be a function of the polar angle $\theta$. However, the ideal blackbody radiation source is assumed to be a Lambertian source, that is, a diffuse emitter of radiation, meaning the direction distribution of released radiation follows the cosine law. This cosine term exactly cancels out the cosine term appearing in the denominator of Equation 3-8. Therefore the spectral emittance of an ideal blackbody radiation source is independent of the viewing angle.

In terms of the spectral emittance, the spectral exitance is

$$M_{e,\lambda}^{b}(\lambda, T) \;=\; \int_{\Omega} L_{e,\lambda}^{b}(\lambda, T)\cos\theta\, d\Omega$$

where the integration is over the half-space (hemisphere) into which the surface area element emits radiation. Since the differential solid angle element in spherical polar coordinates is

$$d\Omega \;=\; \sin\theta\, d\theta\, d\phi$$

the relationship between spectral emittance and spectral exitance becomes

$$M_{e,\lambda}^{b}(\lambda, T) \;=\; \int_{0}^{2\pi}\int_{0}^{\pi/2} L_{e,\lambda}^{b}(\lambda, T)\sin\theta\cos\theta\, d\theta\, d\phi \;=\; \pi L_{e,\lambda}^{b}(\lambda, T)$$

Or alternatively,

$$L^b_{e,\lambda}(\lambda, T) = \frac{1}{\pi}M^b_{e,\lambda}(\lambda, T)$$

Although any differential area on the surface of the blackbody releases radiation into the hemispherical half-space above it (subtending a solid angle of $2\pi$ steradians), the conversion between exitance and radiance only requires a multiplication by $\pi$ rather than $2\pi$. This has been shown in the above derivation to follow from the treatment of an ideal blackbody as a Lambertian source.

### PLANCK'S LAW OF BLACKBODY RADIATION

The spectral exitance of an ideal blackbody radiation source follows Planck's law. In terms of the wavelength,

$$M^b_{e,\lambda}(\lambda, T) = \frac{2\pi hc^2}{\lambda^5}\left[\exp\left(\frac{hc}{k_B\lambda T}\right) - 1\right]^{-1} \tag{3-9}$$

Or in terms of the frequency,

$$M^b_{e,\nu}(\nu, T) = \frac{2\pi h\nu^3}{c^2}\left[\exp\left(\frac{h\nu}{k_B T}\right) - 1\right]^{-1} \tag{3-10}$$

Similarly, the spectral radiance may be expressed as a function of wavelength or frequency,

$$L^b_{e,\lambda}(\lambda, T) = \frac{2hc^2}{\lambda^5}\left[\exp\left(\frac{hc}{k_B\lambda T}\right) - 1\right]^{-1}$$

$$L^b_{e,\nu}(\nu, T) = \frac{2h\nu^3}{c^2}\left[\exp\left(\frac{h\nu}{k_B T}\right) - 1\right]^{-1}$$

*Dismissing an Apparent Paradox*

One might be inclined to substitute $\lambda = c/\nu$ into Equation 3-9 or substitute $\nu = c/\lambda$ into Equation 3-10. Doing so would give seemingly contradictory expressions for the spectral exitance, but doing so would be a mistake because the exitance is not energy flux itself but rather a distribution function of the energy flux (Ref. 7). A better comparison is to integrate Equation 3-9 and Equation 3-10 over matching wavelength and frequency ranges, respectively, noting from Equation 3-7 that these integrals should agree.

$$\int_{\lambda_1}^{\lambda_2} M_{e,\lambda}^b(\lambda, T)d\lambda = \int_{\lambda_1}^{\lambda_2} \frac{2\pi hc^2}{\lambda^5}\left[\exp\left(\frac{hc}{k_B\lambda T}\right) - 1\right]^{-1}d\lambda$$

$$\int_{\nu_2}^{\nu_1} M_{e,\nu}^b(\nu, T)d\nu = \int_{\nu_2}^{\nu_1} \frac{2\pi h\nu^3}{c^2}\left[\exp\left(\frac{h\nu}{k_B T}\right) - 1\right]^{-1}d\nu$$

Then in the first integral, the following substitutions are made:

$$\lambda = \frac{c}{\nu} \qquad d\lambda = -\frac{c}{\nu^2}d\nu \qquad \lambda_1 = \frac{c}{\nu_1} \qquad \lambda_2 = \frac{c}{\nu_2}$$

The integral then becomes

$$\int_{\lambda_1}^{\lambda_2} M_{e,\lambda}^b(\lambda, T)d\lambda = \int_{\nu_1}^{\nu_2} \frac{2\pi h\nu^5}{c^3}\left[\exp\left(\frac{h\nu}{k_B T}\right) - 1\right]^{-1}\left(-\frac{c}{\nu^2}d\nu\right)$$

Using the negative sign to reverse the limits of integration and then simplifying yields

$$\int_{\lambda_1}^{\lambda_2} M_{e,\lambda}^b(\lambda, T)d\lambda = \int_{\nu_2}^{\nu_1} \frac{2\pi h\nu^3}{c^2}\left[\exp\left(\frac{h\nu}{k_B T}\right) - 1\right]^{-1}d\nu$$

The integrand on the right-hand side matches the original definition of $M_{e,\nu}^b(\nu, T)$, so there is no contradiction. The key takeaway is the following:

> 💡 The spectral exitance and spectral radiance are distribution functions of a spectral variable. Any substitution of a different spectral variable must be accompanied by the appropriate Jacobian of transformation.

This fundamental truth about the nature of spectral exitance is the reason why phenomena such as Wien peaks appear to change location when the exitance is expressed in terms of a different independent variable.

### SAMPLING FROM THE PLANCK DISTRIBUTION

To simulate the emission of radiation from a blackbody radiation source, the wavelength or frequency of a representative population of rays must be sampled from the Planck function. To describe how values might be sampled from this distribution function, it is convenient to introduce the dimensionless variable $x$ (not to be confused with the spatial $x$-coordinate)

$$x = \frac{h\nu}{k_B T} = \frac{hc}{k_B\lambda T}$$

The Jacobian of transformation is

$$\mathrm{d}x = \frac{h}{k_{\mathrm{B}}T}\mathrm{d}v = -\frac{hc}{k_{\mathrm{B}}\lambda^2 T}\mathrm{d}\lambda$$

In terms of this dimensionless variable, the spectral exitance is

$$M_{\mathrm{e},x}^{\mathrm{b}}(x, T) = \frac{2\pi k_{\mathrm{B}}^4 T^4}{h^3 c^2}\frac{x^3}{e^x - 1}$$

And the total exitance is thus

$$M_{\mathrm{e}}^{\mathrm{b}}(T) = \frac{2\pi k_{\mathrm{B}}^4 T^4}{h^3 c^2}\int_0^\infty \frac{x^3}{e^x - 1}\mathrm{d}x$$

It can be shown by taking a series expansion of the integrand and then integrating every term by parts (Ref. 7) that the value of the integral is

$$\int_0^\infty \frac{x^3}{e^x - 1}\mathrm{d}x = \frac{\pi^4}{15}$$

although there is no closed-form expression for this integral if the upper limit of integration is finite; in that case, numerical integration is required. The expression for the total exitance is then

$$M_{\mathrm{e}}^{\mathrm{b}}(T) = \frac{2\pi^5 k_{\mathrm{B}}^4 T^4}{15 h^3 c^2} = \sigma T^4$$

where $\sigma$ is the Stefan-Boltzmann constant,

$$\sigma = \frac{2\pi^5 k_{\mathrm{B}}^4}{15 h^3 c^2} \approx 5.67 \times 10^{-8}\frac{\mathrm{W}}{\mathrm{m}^2 \mathrm{K}^4}$$

Thus an integration of Planck's law confirms the Stefan-Boltzmann law.

It is convenient to normalize the spectral exitance so that it represents a probability distribution function of $x$,

$$f(x) = \frac{15}{\pi^4}\frac{x^3}{e^x - 1}$$

In the COMSOL implementation, when polychromatic radiation is permitted in a model (by selecting either **Polychromatic, specify vacuum wavelength** or **Polychromatic,**

**specify frequency** from the physics interface **Wavelength distribution of released rays** list), values of $x$ are first sampled from the above probability distribution function and then converted to the vacuum wavelength or frequency as needed.

## *Gaussian Beam Theory*

The Gaussian Beam node releases rays with a Gaussian distribution of intensity or power. It can only be used when solving for either intensity or power, or both.

> ⚠️ The Geometrical Optics interface does not consider diffraction effects. Therefore, using the **Gaussian Beam** node involves two key assumptions:
>
> - The distances the rays propagate in the model should either be much larger than or much smaller than the Rayleigh range of the beam, which will be defined in a later section.
>   - For ray propagation over relatively short distances, choose **Collimated source (large Rayleigh range)** from the **Beam type** list.
>   - For ray propagation over relatively large distances, choose **Point source (small Rayleigh range)** from the **Beam type** list.
> - Paraxial approximation: the beam divergence angle should be small.

### EFFECT OF SPACE DIMENSION

The **Gaussian Beam** node is available in 3D, 2D axisymmetric, and 2D geometries. The interpretation of the beam is different in 2D than in 3D or 2D axisymmetric models.

- In 3D, the beam irradiance distribution is assumed to be rotationally symmetric about the beam axis, the average direction of the released rays. The beam axis may be in any arbitrary direction.

- In 2D axisymmetric models, the irradiance distribution is still assumed to be rotationally symmetric about the beam axis, but the beam axis is restricted to either the positive or negative $z$ direction. If any other direction were chosen as the beam axis, the beam would not actually be Gaussian in the corresponding 3D solid of revolution.

- In 2D models, the irradiance distribution exhibits plane symmetry across the beam axis but is uniform in the out-of-plane direction. Thus in the vicinity of the beam waist, the beam appears more as a sheet rather than a cylinder.

## GAUSSIAN BEAM EQUATION IN 3D

Without loss of generality we assume the beam is propagating in the positive $z$ direction with a waist centered at the origin, although in a 3D geometry any other waist position and beam axis may be specified.

The electric field amplitude of a paraxial Gaussian beam is most conveniently expressed in cylindrical polar coordinates,

$$\mathbf{E}(\rho, z) = \mathbf{E}_0 \frac{w_0}{w(z)} \exp\left[ -\frac{\rho^2}{w(z)^2} - jkz - jk\frac{\rho^2}{2R(z)} + j\eta(z) \right] \qquad (3\text{-}11)$$

where

- $\rho$ (SI unit: m) is the radial coordinate (with the beam centered around $\rho = 0$),
- $z$ (SI unit: m) is the axial coordinate (chosen so that $z = 0$ is the beam waist),
- $\mathbf{E}(\rho,z)$ (SI unit: V/m) is the electric field at an arbitrary location $(\rho,z)$,
- $\mathbf{E}_0 = \mathbf{E}(0,0)$ is the electric field at the center of the beam waist, and
- $k$ (SI unit: rad/m) is the wave number in the medium through which the beam propagates, $k = 2\pi/\lambda = 2\pi n/\lambda_0$ where $n$ (dimensionless) is the absolute refractive index of the medium and $\lambda_0$ (SI unit: m) is the vacuum wavelength.

The beam parameter $w_0$ is called the waist radius. Of course, there is no well-defined cutoff distance at which the electric field goes to zero, so there is a certain degree of arbitrariness involved in assigning a value to the beam radius. As will be shown in the following sections, the beam waist radius is defined such that the fraction of the total beam power that passes through a circle or radius $w_0$ centered at the origin is $1 - e^{-2}$.

The remaining functions in Equation 3-11 are defined as follows:

The function $w(z)$ is the beam radius at any axial coordinate $z$,

$$w = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2}$$

The function $R(z)$ describes how quickly the beam phase varies with radial position in a plane located at any axial coordinate $z$,

$$R(z) = z\left[ 1 + \left(\frac{z_R}{z}\right)^2 \right]$$

The term $\eta(z)$ is an additional phase delay known as the Guoy phase,

$$\eta(z) = \mathrm{atan}\left(\frac{z}{z_R}\right)$$

In these definitions, $z_R$ (SI unit: m) is the Rayleigh range,

$$z_R = \frac{\pi w_0^2}{\lambda}$$

The Rayleigh range is the axial distance from the beam waist at which the radius has increased by a factor of $\sqrt{2}$, or equivalently the distance from the beam waist at which the cross sectional area of the beam has doubled.

The exponent in Equation 3-11 can be separated into amplitude and phase terms,

$$\mathbf{E}(\rho, z) = \mathbf{E}_0 \frac{w_0}{w(z)} \exp\left[-\frac{\rho^2}{w(z)^2}\right] \exp[-j\delta]$$

where $\delta$ (SI unit: rad) is the phase factor,

$$\delta = kz + k\frac{\rho^2}{2R(z)} - \eta(z) \tag{3-12}$$

### GAUSSIAN BEAM EQUATION FOR IRRADIANCE

It is also possible to write Equation 3-11 in terms of the irradiance rather than electric field amplitude. As the irradiance $I$ (SI unit: $\mathrm{W/m^2}$) is proportional to $\mathbf{E} \cdot \mathbf{E}^*$, the phase factor vanishes,

$$I(\rho, z) = I_0 \left(\frac{w_0}{w(z)}\right)^2 \exp\left(-2\frac{\rho^2}{w(z)^2}\right) \tag{3-13}$$

### ASYMPTOTIC LIMITS OF THE PARAXIAL GAUSSIAN BEAM

In the asymptotic limit as the $z$-coordinate is much greater than the Rayleigh range, the beam radius approaches a linear function of $z$,

$$w(z) = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2} \approx w_0 \frac{z}{z_R} \qquad |z| \gg z_R$$

so a beam with radius $w(z)$ approaches a biconical shape (with both cone vertices meeting at the origin) in the limits $z \ll -z_R$ and $z \gg z_R$. These asymptotes each make an angle of $\alpha$ (SI unit: rad) with the beam axis, where

$$\alpha = \frac{\lambda}{\pi w_0}$$

$\alpha$ is called the beam divergence half-angle, to avoid confusion with references such as Ref. 8 that may define a full angle equal to $2\alpha$.

Making the substitution $w(z) \approx w_0 z / z_R$ into Equation 3-13 then yields

$$I(\rho, z) = I_0 \left(\frac{z_R}{z}\right)^2 \exp\left[-2\left(\frac{z_R}{w_0}\right)^2\left(\frac{\rho}{z}\right)^2\right]$$

At this point it is convenient to convert to spherical polar coordinates,

$$\rho = r \sin\theta \qquad z = r \cos\theta$$

where $r$ (SI unit: m) is the distance from the origin and $\theta$ (SI unit: rad) is the polar angle measured from the positive $z$-axis. Thus

$$I(r, \theta) = I_0 \left(\frac{z_R}{r \cos\theta}\right)^2 \exp\left[-2\left(\frac{z_R}{w_0}\right)^2\left(\frac{r \sin\theta}{r \cos\theta}\right)^2\right]$$

Note also from the definitions of the Rayleigh range and the divergence half-angle that

$$\alpha = \frac{w_0}{z_R}$$

Thus

$$I(r, \theta) = I_0 \left(\frac{z_R}{r \cos\theta}\right)^2 \exp\left[-2\left(\frac{\tan\theta}{\alpha}\right)^2\right]$$

Finally, recall that the Gaussian beam is paraxial (small $\theta$). Taylor series expansions of the cosine and tangent functions reveal that

$$\tan\theta = \theta + O(\theta^3)$$
$$\cos\theta = 1 + O(\theta^2)$$

So that for small $\theta$,

$$I(r, \theta) = I_0 \left(\frac{z_R}{r}\right)^2 \exp\left[-2\left(\frac{\theta}{\alpha}\right)^2\right] \tag{3-14}$$

Equation 3-14 shows that the far-field limit of a Gaussian beam ($z \gg z_R$) is a cone of half-angle $\alpha$ in which the ray intensity or power is proportional to a Gaussian function of the angle between each ray and the beam axis.

### ASYMPTOTIC LIMIT OF PHASE

The Geometrical Optics interface includes the option to treat rays as fully coherent wavefronts in which the instantaneous phase is solved for, by selecting the **Compute phase** check box. When the rays are treated as a collimated source, their phase is initialized as if all rays are released at locations along the beam waist. Substituting $z = 0$ into Equation 3-12 for the phase factor simply yields $\delta = 0$, so the initial phase of all released rays is equal.

Now consider once again the asymptotic limit of $z \gg z_R$.

$$w(z) = w_0 \sqrt{1 + \left(\frac{z}{z_R}\right)^2} \approx w_0 \frac{z}{z_R}$$

$$R(z) = z\left[1 + \left(\frac{z_R}{z}\right)^2\right] \approx z$$

$$\lim_{z \to \infty} \operatorname{atan}\left(\frac{z}{z_R}\right) = \frac{\pi}{2}$$

So for large $z$, Equation 3-12 becomes

$$\delta = kz + k\frac{\rho^2}{2z} - \frac{\pi}{2}$$

Again converting to spherical polar coordinates,

$$\delta = kr\cos\theta + \frac{1}{2}kr\sin\theta\tan\theta - \frac{\pi}{2}$$

And in fact a Taylor series expansion shows that

$$\cos\theta + \frac{1}{2}\sin\theta\tan\theta = 1 + \frac{1}{8}\theta^4 + \frac{1}{24}\theta^6 + O(\theta^8)$$

So the phase of the released rays can be considered uniform, so long as

$$kL\theta^4 \ll 1$$

where $L$ is the maximum distance the rays propagate in the model.

### TOTAL BEAM POWER AND ENCIRCLED POWER

The total power transmitted by the Gaussian beam $P_{src}$ (SI unit: m) is found by integrating the irradiance from Equation 3-13 over a plane perpendicular to the $z$-axis,

$$P_{src} = \int_0^{2\pi} \int_0^{\infty} I_0 \left(\frac{w_0}{w(z)}\right)^2 \exp\left(-2\frac{\rho^2}{w(z)^2}\right) \rho d\rho d\phi = \frac{\pi}{2} w_0^2 I_0$$

As expected, the total power crossing a plane perpendicular to the $z$-axis does not depend on the value of $z$, otherwise energy would be accumulating at some location in the beam.

Compare the total source power $P_{src}$ with the encircled power $P_{cir}$ (SI unit: W/m$^2$) that passes through a circle of radius $w(z)$ centered at the $z$-axis,

$$P_{cir} = \int_0^{2\pi} \int_0^{w(z)} I_0 \left(\frac{w_0}{w(z)}\right)^2 \exp\left(-2\frac{\rho^2}{w(z)^2}\right) \rho d\rho d\phi = \frac{\pi}{2} w_0^2 I_0 (1 - e^{-2})$$

Thus the radio of the encircled power to the total source power is

$$\frac{P_{cir}}{P_{src}} = 1 - e^{-2} \approx 0.865$$

In addition, by substituting $\rho = 0$ and $\rho = w(z)$ into Equation 3-13, it follows that

$$\frac{I(w(z), z)}{I(0, z)} = e^{-2}$$

Thus the beam radius $w(z)$ is sometimes called the $1/e^2$ radius. If the above integral is repeated, replacing the upper limit integration with $cw(z)$ where $c$ is a positive constant (called the **Beam cutoff ratio** in the settings window), the result is

$$P_{cir} = \int_0^{2\pi} \int_0^{cw(z)} I_0 \left(\frac{w_0}{w(z)}\right)^2 \exp\left(-2\frac{\rho^2}{w(z)^2}\right) \rho d\rho d\phi = \frac{\pi}{2} w_0^2 I_0 [1 - \exp(-2c^2)]$$

### SUMMARY OF BEAM PARAMETERS (3D)

When the wavelength of the beam $\lambda$ and any one of the three beam parameters (waist radius $w_0$, divergence half-angle $\alpha$, and Rayleigh range $z_R$) are defined, the other two beam parameters can be derived:

$$w_0 = \frac{\lambda}{\pi\alpha} = \sqrt{\frac{z_R\lambda}{\pi}}$$

$$\alpha = \frac{\lambda}{\pi w_0} = \sqrt{\frac{\lambda}{\pi z_R}}$$

$$z_R = \frac{w_0}{\alpha} = \frac{\lambda}{\pi\alpha^2} = \frac{\pi w_0^2}{\lambda}$$

For a beam of given waist radius $w_0$ and any of the three intensity-related parameters (intensity at the beam waist $I_0$, total source power $P_{src}$ or encircled power $P_{cir}$), the remaining two parameters can be derived:

$$I_0 = \frac{2P_{src}}{\pi w_0^2} = \frac{2P_{cir}}{\pi w_0^2}[1 - \exp(2c^2)]^{-1}$$

$$P_{src} = \frac{\pi}{2}w_0^2 I_0 = P_{cir}[1 - \exp(2c^2)]^{-1}$$

$$P_{cir} = P_{src}[1 - \exp(2c^2)] = \frac{\pi}{2}w_0^2 I_0[1 - \exp(2c^2)]$$

### GAUSSIAN BEAM EQUATION IN 2D

The Gaussian beam in 2D has a different functional form because instead of having rotational symmetry about the beam axis, it is uniform in the out-of-plane direction,

$$\mathbf{E}(x,y) = \mathbf{E}_0 \sqrt{\frac{w_0}{w(x)}} \exp\left[-\frac{y^2}{w(x)^2} - jkx - jk\frac{y^2}{2R(x)} + j\eta(x)\right]$$

$$w(x) = w_0\sqrt{1 + \left(\frac{x}{z_R}\right)^2} \qquad R(x) = x\left[1 + \left(\frac{z_R}{x}\right)^2\right] \qquad \eta(x) = \frac{1}{2}\text{atan}\left(\frac{x}{z_R}\right)$$

Comparing the 2D form with the 3D form from Equation 3-11, the key differences are a square root on the term $w_0/w(x)$ and a factor of $1/2$ in the Guoy phase. In this expression $x$ has been considered the propagation direction but the beam may actually propagate in any direction in the $xy$-plane.

The corresponding expression for the beam irradiance is

$$I(x,y) = I_0\frac{w_0}{w(x)}\exp\left[-2\frac{y^2}{w(x)^2}\right]$$

The total beam power per unit distance in the out-of-plane direction is

$$\frac{P_{src}}{\Delta z} = \int_{-\infty}^{\infty} I_0 \frac{w_0}{w(x)} \exp\left[-2\frac{y^2}{w(x)^2}\right] dy = I_0 w_0 \sqrt{\frac{\pi}{2}}$$

The 2D analogue to the encircled power from the previous section, the beam power per unit distance that passes between coordinates $-cw(x)$ and $cw(x)$ is

$$\frac{P_{cir}}{\Delta z} = \int_{-cw(x)}^{cw(x)} I_0 \frac{w_0}{w(x)} \exp\left[-2\frac{y^2}{w(x)^2}\right] dy$$

Because the irradiance is an even function of $y$, this may be simplified to

$$\frac{P_{cir}}{\Delta z} = 2I_0 \int_{0}^{cw(x)} \frac{w_0}{w(x)} \exp\left[-2\frac{y^2}{w(x)^2}\right] dy = I_0 w_0 \sqrt{\frac{\pi}{2}} \mathrm{erf}(\sqrt{2}c)$$

Thus the ratio of the encircled power to the total source power is

$$\frac{P_{cir}}{P_{src}} = \mathrm{erf}(\sqrt{2}c)$$

where the error function `erf` is a built-in function in COMSOL,

$$\mathrm{erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_{0}^{x} \exp(-x'^2) dx'$$

For $c = 1$ the encircled power is about 95% of the total beam power.

## Material Discontinuity Theory

At a Material Discontinuity between two different media, the wave vector is reinitialized using Snell's law. First, the angle of incidence $\theta_i$ is computed:

$$\theta_i = \mathrm{acos}\left(\frac{\mathbf{n}_i \cdot \mathbf{n}_s}{|\mathbf{n}_i||\mathbf{n}_s|}\right)$$

where $\mathbf{n}_i$ is a unit vector in the direction of the incident ray and $\mathbf{n}_s$ is a unit vector normal to the material discontinuity.

At a boundary between two isotropic, nonabsorbing media, the refracted ray propagates in the direction $\mathbf{n}_t$ given by the following relations:

$$\mathbf{n}_t = \eta \mathbf{n}_i + \gamma \mathbf{n}_s$$

$$\gamma = -\eta \cos\theta_i + \cos\theta_t$$

$$\eta = \frac{n_1}{n_2}$$

$$\theta_t = \text{asin}(\eta \sin\theta_i)$$

where the ray propagates from the medium with refractive index $n_1$ into the medium with refractive index $n_2$. Because the two media are nonabsorbing, the quantities $n_1$, $n_2$, $\theta_i$, and $\theta_t$ are real-valued. If the media are weakly absorbing, the real parts of $n_1$ and $n_2$, are used. If the media are strongly absorbing, several corrections to Snell's law and the Fresnel equations must be made, as discussed in Refraction in Strongly Absorbing Media.

If the maximum number of secondary rays has not yet been released, a reflected ray is also released at the material discontinuity with the initial direction

$$\mathbf{n}_r = \mathbf{n}_i - 2\mathbf{n}_s \cos\theta_i$$

If the ray intensity is computed, the release of secondary rays may be suppressed when the intensity of the reflected ray is less than the user-defined **Threshold intensity** $I_{th}$ (SI unit: W/m$^2$). Similarly, when ray power is computed, a **Threshold power** $Q_{th}$ (SI unit: W) can be specified.

*The Fresnel Equations*

At a boundary between two media, the tangential components of the electric field **E** are conserved. If there are no surface currents, the tangential components of the magnetic field **H** are also conserved.

If the incident ray is s-polarized, meaning the electric field is perpendicular to the plane of incidence, then from the conservation of the tangential components of **E** and **H**,

$$E_{st} = E_{si} + E_{sr} \tag{3-15}$$

$$n_2 E_{st} \cos\theta_t = n_1 (E_{si} - E_{sr}) \cos\theta_i \tag{3-16}$$

Substitution of Equation 3-16 into Equation 3-15 yields the ratios

$$\frac{E_{sr}}{E_{si}} = \frac{n_1 \cos\theta_i - n_2 \cos\theta_t}{n_1 \cos\theta_i + n_2 \cos\theta_t} \qquad \frac{E_{st}}{E_{si}} = \frac{2n_1 \cos\theta_i}{n_1 \cos\theta_i + n_2 \cos\theta_t}$$

Similarly, if the incident ray is p-polarized, meaning that the electric field lies in the plane of incidence and the magnetic field lies perpendicular to it, then from the conservation of the tangential components of **E** and **H**,

$$E_{pt}\cos\theta_t = (E_{pi} - E_{pr})\cos\theta_i \qquad (3\text{-}17)$$

$$n_2 E_{pt} = n_1(E_{pi} - E_{pr}) \qquad (3\text{-}18)$$

Substitution of Equation 3-18 into Equation 3-17 yields the ratios

$$\frac{E_{pr}}{E_{pi}} = \frac{n_2\cos\theta_i - n_1\cos\theta_t}{n_2\cos\theta_i + n_1\cos\theta_t} \qquad \frac{E_{pt}}{E_{pi}} = \frac{2n_1\cos\theta_i}{n_2\cos\theta_i + n_1\cos\theta_t}$$

Finally, we define the reflection coefficient as the ratio of the reflected electric field amplitude to the incident electric field amplitude, and similarly define the transmission coefficient as the ratio of the refracted electric field amplitude to the incident electric field amplitude.

$$r_p = \frac{n_2\cos\theta_i - n_1\cos\theta_t}{n_2\cos\theta_i + n_1\cos\theta_t} \qquad t_p = \frac{2n_1\cos\theta_i}{n_2\cos\theta_i + n_1\cos\theta_t}$$

$$r_s = \frac{n_1\cos\theta_i - n_2\cos\theta_t}{n_1\cos\theta_i + n_2\cos\theta_t} \qquad t_s = \frac{2n_1\cos\theta_i}{n_1\cos\theta_i + n_2\cos\theta_t}$$

The above definition of $r_p$ is consistent with Ref. 9 but shows the opposite sign compared to Ref. 10. This is because Ref. 9 defines the direction of the in-plane field component such that the s-polarized component, p-polarized component, and ray direction vector (in that order) always comprise a right-handed coordinate system; whereas in Ref. 10 the vectors written in this order would comprise a left-handed coordinate system for the reflected ray.

## *Intensity, Wavefront Curvature, and Polarization*

The following describes the algorithm used to compute the ray intensity and polarization when **Intensity computation** is set to **Compute intensity** or **Compute intensity and power** in the physics interface **Intensity Computation** section. In this algorithm, each ray is treated as a propagating wavefront subtending a small solid angle. The algorithm is only valid when the rays propagate in homogeneous media. The following auxiliary dependent variables are defined for each ray:

In 3D:

- The initial ray intensity $I_0$ and normalized Stokes parameters $s_{n1}$, $s_{n2}$, and $s_{n3}$. By allocating four degrees of freedom in this way it is possible to characterize any intensity magnitude and polarization state.

- The integral $A$ of the attenuation coefficient along the ray path.

- Two initial principal radii of curvature, $r_{1,i}$ and $r_{2,i}$.

- Two principal radii of curvature, $r_1$ and $r_2$, which represent the maximum and minimum radii of curvature of the intersection of the wavefront with an arbitrary plane.

- Three components of a unit vector $\mathbf{e}_1$ in the direction corresponding to the first principal radius of curvature. This information is used to reinitialize the principal radii of curvature at curved boundaries.

In 2D:

- The initial ray intensity $I_0$ and normalized Stokes parameters $s_{n1}$, $s_{n2}$, and $s_{n3}$.

- The integral $A$ of the attenuation coefficient along the ray path.

- One initial principal radius of curvature, $r_{1,i}$.

- One radius of curvature $r_1$ of the wavefront. All wavefronts are assumed to be converging or diverging cylindrical waves, so it is not necessary to define a second radius of curvature.

A different algorithm is used to compute the intensity and polarization of each ray if the **Intensity computation** is instead set to **Compute intensity in graded media** or **Compute intensity and power in graded media**. This algorithm accounts for the effect of graded media on the ray intensity, but it is also slower and less accurate for homogeneous media. The following auxiliary dependent variables are defined for each ray:

In 3D:

- The intensity help variable $\Gamma$ and the normalized Stokes parameters $s_{n01}$, $s_{n02}$, and $s_{n03}$, which characterize the intensity and polarization of the ray. They are reinitialized at material discontinuities and walls.

- The integral $A$ of the attenuation coefficient along the ray path.

- Two principal curvature calculation help variables $\alpha_1$ and $\alpha_2$ and the rotation angle $\phi$ which indicates the orientation of the principal curvature directions. An additional help variable is used internally to detect poles in the local coordinate system definition and to redefine the local coordinate system accordingly.

In 2D:

- The intensity help variable $\Gamma$ and the normalized Stokes parameters $s_{n01}$, $s_{n02}$, and $s_{n03}$, which characterize the intensity and polarization of the ray. They are reinitialized at material discontinuities and walls.

- The integral $A$ of the attenuation coefficient along the ray path.

- One principal curvature calculation help variable $\alpha_1$.

For the options **Compute Power**, **Compute intensity and power**, and **Compute intensity and power in graded media** an additional auxiliary dependent variable is defined to indicate the total power transmitted by each ray. Like intensity, power is affected by absorbing media and by reflection or refraction at boundaries. Unlike intensity, power does not change due to the focusing or divergence of a ray bundle.

### THE STOKES PARAMETERS

The four Stokes parameters completely characterize the intensity and polarization of a fully polarized, partially polarized, or unpolarized ray. The Stokes parameters can be interpreted as indicators of the ray intensity that would be measured when sending a ray through various arrangements of polarizers and wave retarders.

The Stokes parameters of a ray are defined as in Ref. 9 as follows. Consider a ray propagating along the $z$-axis of a Cartesian coordinate system, with electric field components polarized within the $xy$-plane. In 3D models the $x$-axis is parallel to the first principal curvature direction $\mathbf{e}_1$. In 2D models the $x$-axis is always oriented in the out-of-plane direction.

Let $I(\theta,\varepsilon)$ be the intensity of radiation polarized in the $xy$-plane at an angle $\theta$ counterclockwise from the $x$-axis, when a phase angle of $\varepsilon$ is introduced between the $x$- and $y$-components. For example, $I(0,0)$ is the intensity that would be measured after sending a ray through a linear polarizer with a transmission axis parallel to the $x$-axis, and $I(\pi/4, \pi/2)$ is the intensity that would be measured after sending a ray through a system of polarizers and wave retarders that only transmits radiation with right-handed circular polarization. The four Stokes parameters are then defined as follows:

- $s_0 = I(0, 0) + I(\pi/2, 0)$ is the sum of the intensity of linearly polarized light in the $x$ and $y$ directions. It represents the total intensity of the ray.

- $s_1 = I(0, 0) - I(\pi/2, 0)$ is the difference in intensity between light that is linearly polarized in the $x$ direction and light that is linearly polarized in the $y$ direction.

- $s_2 = I(\pi/4, 0) - I(3\pi/4, 0)$ is the difference in intensity between linearly polarized light in the direction of the line $y = x$ and linearly polarized light in the direction of the line $y = -x$.

- $s_3 = I(\pi/4, \pi/2) - I(3\pi/4, \pi/2)$ is the difference in intensity between light with right-handed circular polarization and light with left-handed circular polarization.

For example, a ray with linear polarization parallel to the $x$-axis has Stokes parameters $s_0 = s_1 = I$ and $s_2 = s_3 = 0$. A fully polarized ray is characterized by the relation

$$s_0^2 = s_1^2 + s_2^2 + s_3^2$$

A partially polarized or unpolarized ray is characterized by the relation

$$s_0^2 \geq s_1^2 + s_2^2 + s_3^2$$

The degree of polarization $P$ is defined as

$$P = \frac{\sqrt{s_1^2 + s_2^2 + s_3^2}}{s_0}$$

A degree of polarization $P = 1$ corresponds to fully polarized radiation, whereas a degree of polarization $P = 0$ corresponds to unpolarized radiation.

In the COMSOL implementation of ray intensity calculation, the degrees of freedom are not the Stokes parameters themselves, but rather normalized Stokes parameters $s_{n1}$, $s_{n2}$, and $s_{n3}$. Then the actual Stokes parameters are recovered through the relations $s_1 = Is_{n1}$, $s_2 = Is_{n2}$, and $s_3 = Is_{n3}$. The reason for this decoupling is that the normalized Stokes parameters remain bounded, enabling accurate reinitialization of ray power, even if a ray is reflected or refracted very close to a caustic, where the intensity (in the geometrical optics limit) can become arbitrarily large.

### PRINCIPAL RADII OF CURVATURE

In 3D models, each ray is treated as a wavefront for which two principal radii of curvature, $r_1$ and $r_2$, are defined. In addition, the values of the two principal radii of curvature are stored as $r_{1,i}$ and $r_{2,i}$ whenever the ray reaches a boundary.

Within domains, the equations

$$\frac{dr_1}{ds} = -1 \qquad \frac{dr_2}{ds} = -1$$

are solved. Negative radii of curvature indicate that the wavefront is expanding as the ray propagates, while positive radii of curvature indicate that the wavefront is converging. A continuous locus of points at which either of the principal radii of curvature equals zero is called a caustic surface. The unit vector $\mathbf{e}_1$ is defined so that $r_1$ is the radius of curvature of the intersection of the wavefront with the plane tangent to $\mathbf{e}_1$ and the wave vector $\mathbf{k}$. Similarly, if a vector $\mathbf{e}_2$ is defined so that

$$\mathbf{e}_2 = \frac{\mathbf{k} \times \mathbf{e}_1}{|\mathbf{k} \times \mathbf{e}_1|}$$

Then $r_2$ is the radius of curvature of the intersection of the wavefront with a plane tangent to $\mathbf{e}_2$ and $\mathbf{k}$. The components of $\mathbf{e}_1$ are stored as auxiliary dependent variables for each ray. The components of $\mathbf{e}_2$ can then be derived from $\mathbf{e}_1$ and $\mathbf{k}$ at any time.

The principal radii of curvature are reinitialized at material discontinuities, and the orientation of the unit vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ may change. If the unit vector in the direction of the incident ray $\mathbf{n}_i$ is not parallel to the surface normal $\mathbf{n}_s$, then it is possible to define a unique tangent plane, called the plane of incidence, that contains the incident, reflected, and refracted rays. The unit vector normal to this plane, $\mathbf{u}_0$, is defined as

$$\mathbf{u}_0 = \frac{\mathbf{n}_i \times \mathbf{n}_s}{|\mathbf{n}_i \times \mathbf{n}_s|}$$

If the ray is normal to the surface, then the incident ray is parallel to the refracted ray and antiparallel to the reflected ray, and $\mathbf{u}_0$ can be any arbitrary unit vector orthogonal to $\mathbf{n}_i$. In addition to the unit vector normal to the plane of incidence, the following unit vectors tangent to the incident wavefront, refracted wavefront, reflected wavefront, and surface normal are defined:

$$\mathbf{u}_i = \mathbf{n}_i \times \mathbf{u}_0$$
$$\mathbf{u}_t = \mathbf{n}_t \times \mathbf{u}_0$$
$$\mathbf{u}_r = \mathbf{n}_r \times \mathbf{u}_0$$
$$\mathbf{u}_s = \mathbf{n}_s \times \mathbf{u}_0$$

where the subscripts $i$, $t$, and $r$ denote the incident, refracted, and reflected wavefronts, respectively. For a wavefront propagating in a direction $\mathbf{n}$, with principal curvatures $k_1 = 1/r_1$ and $k_2 = 1/r_2$ defined for directions $\mathbf{e}_1$ and $\mathbf{e}_2$, the principal curvatures in two other orthogonal directions $\mathbf{e}_1{}'$ and $\mathbf{e}_2{}'$ (both orthogonal to $\mathbf{n}$) are

$$k_1' = k_1\cos^2\theta + k_2\sin^2\theta \qquad\qquad (3\text{-}19)$$
$$k_2' = k_1\sin^2\theta + k_2\cos^2\theta$$
$$k_{12}' = (k_1 - k_2)\cos\theta\sin\theta$$

where $\theta$ is the angle of rotation about $\mathbf{n}$ which transforms the vectors $\mathbf{e}_1$ and $\mathbf{e}_2$ to $\mathbf{e}_1'$ and $\mathbf{e}_2'$, respectively. Because $k_1'$ and $k_2'$ are not principal curvatures, it is necessary to include off-diagonal elements of the wavefront curvature tensor equal to $k_{12}'$.

The following algorithm is used to reinitialize the principal radii of curvature of the wavefront and their orientations. The reinitialization of the curvature variables follows the method of Stavroudis in Ref. 11.

**1** Given $\mathbf{n}_i$ and $\mathbf{n}_s$, compute unit vectors in the directions of the reflected and refracted rays, $\mathbf{n}_r$ and $\mathbf{n}_t$.

**2** Compute the vectors $\mathbf{u}_0$, $\mathbf{u}_i$, $\mathbf{u}_t$, $\mathbf{u}_r$, and $\mathbf{u}_s$.

**3** Compute the angle of rotation $\theta^{(i)}$ needed to transform the local coordinate system with axes parallel to $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{n}_i$ to a local coordinate system with axes parallel to $\mathbf{u}_0$, $\mathbf{u}_i$, and $\mathbf{n}_i$. (Note: the superscript $^{(i)}$ is used to distinguish this coordinate system rotation angle from the angle of incidence of the ray, often denoted $\theta_i$.)

**4** Transform the principal curvatures to the local coordinate system defined by $\mathbf{u}_0$, $\mathbf{u}_i$, and $\mathbf{n}_i$ by using Equation 3-19, substituting $\theta^{(i)}$ for $\theta$.

**5** Given the two principal curvatures of the surface, $k_{1,s}$ and $k_{2,s}$ with directions $\mathbf{e}_{1,s}$ and $\mathbf{e}_{2,s}$, transform the curvature variables to a local coordinate system with axes parallel to $\mathbf{u}_0$, $\mathbf{u}_s$, and $\mathbf{n}_s$. Let the new curvature variables be denoted by $k_{1,s}'$, $k_{2,s}'$, and $k_{12,s}'$.

**6** The curvatures of the wavefront and the surface have now been defined in coordinate systems that share the axis $\mathbf{u}_0$ and only differ by a rotation by the angle of incidence $\theta_i$ about $\mathbf{u}_0$. Defining the variables $\eta$ and $\gamma$ as in Material Discontinuity Theory, compute the curvature variables of the refracted ray in a coordinate system defined by $\mathbf{u}_0$, $\mathbf{u}_t$, and $\mathbf{n}_t$ using the equations

$$k_{1,t}' = \eta k_1' + \gamma k_{1,s}'$$

$$k_{12,t}' = \frac{\eta\cos\theta_i}{\cos\theta_t}k_{12}' + \frac{\gamma}{\cos\theta_t}k_{12,s}'$$

$$k_{2,t}' = \frac{\eta\cos^2\theta_i}{\cos^2\theta_t}k_2' + \frac{\gamma}{\cos^2\theta_t}k_{2,s}'$$

**7** Obtain the principal curvatures of the refracted ray by rotating the coordinate system defined by $\mathbf{u}_0$, $\mathbf{u}_t$, and $\mathbf{n}_t$ by an angle $\theta^{(t)}$ about $\mathbf{n}_t$. The angle $\theta^{(t)}$ is defined as

$$\theta^{(t)} = \frac{1}{2}\operatorname{atan}\left(\frac{2k_{12,\,t}'}{k_{1,\,t}' - k_{2,\,t}'}\right)$$

**8** Reinitialize the principal curvatures of the refracted ray:

$$k_{1,\,t} = k_{1,\,t}'\cos^2\theta^{(t)} + 2k_{12,\,t}'\cos\theta^{(t)}\sin\theta^{(t)} + k_{2,\,t}'\sin^2\theta^{(t)}$$
$$k_{2,\,t} = k_{1,\,t}'\sin^2\theta^{(t)} - 2k_{12,\,t}'\cos\theta^{(t)}\sin\theta^{(t)} + k_{2,\,t}'\cos^2\theta^{(t)}$$

**9** Invert the principal curvatures to obtain the principal radii of curvature of the refracted ray. Rotate $\mathbf{u}_0$ about $\mathbf{n}_t$ by the angle $\theta^{(t)}$ to obtain the reinitialized principal curvature direction $\mathbf{e}_{1,t}$.

**10** If a reflected ray is released, compute the curvature variables of the reflected ray in a coordinate system defined by $\mathbf{u}_0$, $\mathbf{u}_r$, and $\mathbf{n}_r$ using the equations

$$k_{1,\,r}' = k_1' - 2k_{1,\,s}'\cos\theta_i$$

$$k_{12,\,r}' = -k_{12}' + 2k_{12,\,s}'$$

$$k_{2,\,r}' = k_2' - \frac{2}{\cos\theta_i}k_{2,\,s}'$$

**11** Obtain the principal curvatures of the reflected ray by rotating the coordinate system defined by $\mathbf{u}_0$, $\mathbf{u}_r$, and $\mathbf{n}_r$ by an angle $\theta^{(r)}$ about $\mathbf{n}_r$. The angle $\theta^{(r)}$ is defined as

$$\theta^{(r)} = \frac{1}{2}\operatorname{atan}\left(\frac{2k_{12,\,r}'}{k_{2,\,r}' - k_{1,\,r}'}\right)$$

**12** Initialize the principal curvatures of the reflected ray:

$$k_{1,\,r} = k_{1,\,r}'\cos^2\theta^{(r)} + 2k_{12,\,r}'\cos\theta^{(r)}\sin\theta^{(r)} + k_{2,\,r}'\sin^2\theta^{(r)}$$
$$k_{2,\,r} = k_{1,\,r}'\sin^2\theta^{(r)} - 2k_{12,\,r}'\cos\theta^{(r)}\sin\theta^{(r)} + k_{2,\,r}'\cos^2\theta^{(r)}$$

**13** Invert the principal curvatures to obtain the principal radii of curvature of the reflected ray. Rotate $\mathbf{u}_0$ about $\mathbf{n}_r$ by the angle $\theta^{(r)}$ to obtain the initialized principal curvature direction $\mathbf{e}_{1,r}$.

In 2D components, only one principal radius of curvature is computed; each ray is treated as a cylindrical wave. In addition, no auxiliary degrees of freedom for the

principal curvature direction are required because the out-of-plane direction can always be treated as one of the axes of the local coordinate system that defines the orientation of the wavefront.

In 2D axisymmetric model components, radii of curvature are computed for the in-plane direction, that is the $rz$-plane, as well as the out-of-plane or azimuthal directions. During ray-boundary interactions, these radii of curvature are reinitialized as if the ray interacted with a 3D surface of revolution, which may have finite radii of curvature in both the in-plane and out-of-plane directions.

### STOKES VECTOR CALCULATION

The values of the intensity $I$ and normalized Stokes parameters are stored as the auxiliary dependent variables $I_0$, $s_{n1}$, $s_{n2}$, and $s_{n3}$ when a ray is released. These auxiliary variables are updated when the ray hits a boundary. At any point along the ray's trajectory, each Stokes parameter is equal to

$$s_0 = I = I_0 \frac{r_{1, i} r_{2, i}}{r_1 r_2} \qquad s_1 = I s_{n1} \qquad s_2 = I s_{n2} \qquad s_3 = I s_{n3}$$

In 2D, the second principal radius of curvature $r_2$ is treated as an arbitrarily large distance that remains constant for each ray. Because $s_1$ and $s_2$ are based on the differences in intensity between orthogonal polarizations of radiation, a local coordinate system must be defined for the ray. Because auxiliary degrees of freedom have already been allocated for $\mathbf{e}_1$ as explained in Principal Radii of Curvature, a local coordinate system is defined with axes parallel to $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{k}$. The axes parallel to $\mathbf{e}_1$ and $\mathbf{e}_2$ then function as the $x$- and $y$-axes in The Stokes Parameters, respectively.

### STOKES VECTOR REINITIALIZATION

*Reflection and Refraction of S- and P-polarized Rays*
Recall from The Fresnel Equations that the ratios of the electric field amplitudes of the incident, reflected, and refracted rays can be expressed as a set of Fresnel coefficients,

$$r_{\mathrm{p}} = \frac{n_2 \cos \theta_i - n_1 \cos \theta_t}{n_2 \cos \theta_i + n_1 \cos \theta_t} \qquad t_{\mathrm{p}} = \frac{2 n_1 \cos \theta_i}{n_2 \cos \theta_i + n_1 \cos \theta_t}$$

$$r_{\mathrm{s}} = \frac{n_1 \cos \theta_i - n_2 \cos \theta_t}{n_1 \cos \theta_i + n_2 \cos \theta_t} \qquad t_{\mathrm{s}} = \frac{2 n_1 \cos \theta_i}{n_1 \cos \theta_i + n_2 \cos \theta_t}$$

where the subscripts $s$ and $p$ denote $s$- and $p$-polarized rays, or rays with linear polarizations perpendicular to and parallel to the plane of incidence, respectively. The incident ray is assumed to move from a region of refractive index $n_1$ toward a region

of refractive index $n_2$. The angles $\theta_i$ and $\theta_t$ are the angle of incidence and angle of refraction, respectively.

If $n_1 > n_2$ and the angle of incidence exceeds the critical angle $\theta = \mathrm{asin}(n_2/n_1)$, the incident ray undergoes total internal reflection, and the reflected ray has intensity equal to that of the incident ray.

The intensity of the transmitted and reflected waves are related to the intensity of the incident wave $I_i$ by the equations

$$I_r = I_i|r_p|^2 \qquad I_t = \frac{n_2\cos\theta_t}{n_1\cos\theta_i}I_i|t_p|^2$$

for $p$-polarized rays, and

$$I_r = I_i|r_s|^2 \qquad I_t = \frac{n_2\cos\theta_t}{n_1\cos\theta_i}I_i|t_s|^2$$

for $s$-polarized rays. The coefficients being multiplied by the incident ray intensity are called the *reflectance $R$* and *transmittance $T$*:

$$R_p = |r_p|^2 \qquad T_p = \frac{n_2\cos\theta_t}{n_1\cos\theta_i}|t_p|^2$$

$$R_s = |r_s|^2 \qquad T_s = \frac{n_2\cos\theta_t}{n_1\cos\theta_i}|t_s|^2$$

*Phase Shift Calculation for Reflected and Refracted Rays*
Any fully polarized ray can be resolved into a pair of $s$- and $p$-polarized rays, with a phase shift $\delta$ between them. The reflected $s$- and $p$-polarized rays at a material discontinuity may then undergo different phase shifts; this may, for example, cause a linearly polarized incident ray to be yield a reflected ray with elliptical polarization. In addition, a phase shift may be applied to the transmitted ray if one or more Thin Dielectric Film subnodes are added to a Material Discontinuity node. The phase shifts of $s$- and $p$-polarized rays are computed from the complex-valued Fresnel coefficients:

$$\Psi_{p,r} = \arg(r_p) \qquad \Psi_{p,t} = \arg(t_p)$$
$$\Psi_{s,r} = \arg(r_s) \qquad \Psi_{s,t} = \arg(t_s)$$

*Unpolarized and Partially Polarized Rays*
An unpolarized ray has the following properties:

• The instantaneous intensity of the ray changes at random.

- At a given instant in time, the ray has an equal probability of being polarized in any direction orthogonal to the ray trajectory.

- The previous two properties are not affected by the transmission of the ray through a wave retarder or a polarization rotator.

An unpolarized ray has Stokes parameters $s_1 = s_2 = s_3 = 0$.

A partially polarized ray is neither completely deterministic nor completely random. It is characterized by a degree of polarization between 0 and 1.

Often, the ray being reflected or refracted at a boundary is unpolarized or partially polarized; or the polarization direction neither lies in the plane of incidence nor perpendicular to it. In this case, a more general formulation for the new values of the Stokes parameters is needed. The Stokes parameters of the reflected and refracted rays can be expressed in terms of the Stokes parameters of the incident ray, the transmittance or reflectance at the boundary, and the phase delay introduced by the boundary (if any) (Ref. 15):

$$
\begin{bmatrix} s_{0t} \\ s_{1t} \\ s_{2t} \\ s_{3t} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} T_s + T_p & T_s - T_p & 0 & 0 \\ T_s - T_p & T_s + T_p & 0 & 0 \\ 0 & 0 & 2\sqrt{T_s T_p}\cos\delta & 2\sqrt{T_s T_p}\sin\delta \\ 0 & 0 & -2\sqrt{T_s T_p}\sin\delta & 2\sqrt{T_s T_p}\cos\delta \end{bmatrix} \begin{bmatrix} s_0 \\ s_1 \\ s_2 \\ s_3 \end{bmatrix},
$$

$$
\begin{bmatrix} s_{0r} \\ s_{1r} \\ s_{2r} \\ s_{3r} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} R_s + R_p & R_s - R_p & 0 & 0 \\ R_s - R_p & R_s + R_p & 0 & 0 \\ 0 & 0 & -2\sqrt{R_s R_p}\cos\delta & -2\sqrt{R_s R_p}\sin\delta \\ 0 & 0 & 2\sqrt{R_s R_p}\sin\delta & -2\sqrt{R_s R_p}\cos\delta \end{bmatrix} \begin{bmatrix} s_0 \\ s_1 \\ s_2 \\ s_3 \end{bmatrix}
$$

where the subscripts $r$ and $t$ represent reflection and refraction, respectively; and the subscripts $s$ and $p$ indicate the transmittance or reflectance for s- and p-polarized rays.

## Wavefront Curvature Calculation in Graded Media

It is possible to compute the ray intensity by changing **Intensity computation** to **Compute intensity** or **Compute intensity in graded media** in the physics interface **Intensity Computation** section. The options **Compute intensity and power** and **Compute intensity and power in graded media** can also be used to compute intensity, with the only difference being that these options define an additional auxiliary dependent variable

for the total power transferred by the ray. The setting **Compute intensity** is more robust and accurate than **Compute intensity in graded media**, but is only applicable to homogeneous media. The setting **Compute intensity in graded media** can be used for both homogeneous and graded media, but it introduces more numerical error than **Compute intensity**.

### ASSUMPTIONS FOR COMPUTING INTENSITY IN HOMOGENEOUS MEDIA

When **Compute intensity** is selected, the ray intensity is computed along each ray path using the following assumptions:

**1** The wavefront represented by each ray subtends a constant plane angle (2D) or solid angle (3D), which can change only when rays are reflected or refracted at boundaries.

**2** Given the radii of curvature at two positions within the same domain and the intensity at one of these two positions, the intensity at the other position can be computed using the relationship

$$I = I_0 \frac{r_{1,0} r_{2,0}}{r_1 r_2}$$

**3** Except when rays are reflected or refracted at boundaries, the principal radii of curvature change at a constant rate:

$$\frac{dr_1}{ds} = \frac{dr_2}{ds} = -1$$

**4** The principal curvature directions do not change, except when rays are reflected or refracted at boundaries.

These assumptions are not valid in graded media, in which the refractive index changes continuously as a function of position. It is possible for the angle between two different rays to change as they propagate through the medium, so the solid angle subtended by the wavefront is no longer constant. As a result, the ray intensity cannot be expressed using the ratio of initial and final principal radii of curvature.

### CURVATURE TENSOR DEFINITION IN GRADED MEDIA

The calculation of ray intensity in graded media is based on the concept of a curvature tensor $\mathbf{K}$, defined in terms of the principal curvatures $\kappa_1$ and $\kappa_2$ and the corresponding principal curvature directions $\mathbf{e}_1$ and $\mathbf{e}_2$:

$$\mathbf{K} = \kappa_1 \mathbf{e}_1 \mathbf{e}_1^T + \kappa_2 \mathbf{e}_2 \mathbf{e}_2^T$$

Because $\mathbf{e}_1$ and $\mathbf{e}_2$ are orthogonal, it follows that $\kappa_1$ and $\kappa_2$ are eigenvalues of $\mathbf{K}$. It also follows that $\mathbf{K}$ is singular because there is no contribution that is orthogonal to both $\mathbf{e}_1$ and $\mathbf{e}_2$.

The signs of the principal curvatures are chosen so that positive curvature indicates that the wavefront is converging, whereas negative curvature indicates that the wavefront is diverging.

The selection of the coordinate system in which the curvature tensor is defined is crucial. It is convenient to describe the coordinate system so that two of the coordinate axes lie in the plane containing $\mathbf{e}_1$ and $\mathbf{e}_2$, since this reduces the number of nonzero terms in $\mathbf{K}$. Further reduction in the number of nonzero terms can be achieved if $\mathbf{K}$ can be defined in a coordinate system in which $\mathbf{e}_1$ and $\mathbf{e}_2$ are basis vectors. This is possible in 2D because one of the principal curvature directions is always parallel to the out-of-plane direction, but in 3D it is not feasible because the principal curvature directions can change as rays propagate through a graded medium.

In the most general 3D case, the curvature tensor is described using the following symbols, each of which corresponds to a different orthonormal basis:

- $\mathbf{K}_X$: curvature tensor defined in the Cartesian coordinate system with basis vectors $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$.

- $\mathbf{K}_W$: curvature tensor defined in the coordinate system consisting of the two principal curvature directions $\mathbf{e}_1$ and $\mathbf{e}_2$ and the direction of propagation $\mathbf{t}$.

- $\mathbf{K}_S$: curvature tensor defined in a coordinate system in which one basis vector is the direction of propagation $\mathbf{t}$. The other two basis vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ can be determined arbitrarily, as long as they are orthogonal to each other and to $\mathbf{t}$, such that $\mathbf{s}_1 \times \mathbf{s}_2 = \mathbf{t}$. It is more convenient to operate in this coordinate system if the basis vectors can be expressed strictly in terms of $\mathbf{x}$, $\mathbf{y}$, $\mathbf{z}$, and $\mathbf{t}$.

The basis vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ are defined as follows:

$$\mathbf{s}_1 = \frac{\mathbf{t} \times \mathbf{z}}{|\mathbf{t} \times \mathbf{z}|} \qquad \mathbf{s}_2 = \mathbf{t} \times \mathbf{s}_1$$

To avoid poles in the definition of the basis vectors, the following alternative definitions are used when the rays propagate nearly parallel to the $z$-axis:

$$\mathbf{s}_1 = \frac{\mathbf{t} \times \mathbf{x}}{|\mathbf{t} \times \mathbf{x}|} \qquad \mathbf{s}_2 = \mathbf{t} \times \mathbf{s}_1$$

The relationship between $\mathbf{s}_1$, $\mathbf{s}_2$, $\mathbf{e}_1$, and $\mathbf{e}_2$ is given by

$$\mathbf{e}_1 = \mathbf{s}_1 \cos\phi - \mathbf{s}_2 \sin\phi$$

$$\mathbf{e}_2 = \mathbf{s}_1 \sin\phi + \mathbf{s}_2 \cos\phi$$

where the rotation angle $\phi$ is an auxiliary dependent variable that is stored for each ray.

The relationship between $\mathbf{K}_S$ and $\mathbf{K}_W$ is given by

$$\mathbf{K}_S = \mathbf{Q}_0 \mathbf{K}_W \mathbf{Q}_0^T$$

where $\mathbf{Q}_0$ is the rotation matrix:

$$\mathbf{Q}_0 = \begin{bmatrix} \mathbf{s}_1 \cdot \mathbf{e}_1 & \mathbf{s}_1 \cdot \mathbf{e}_2 & \mathbf{s}_1 \cdot \mathbf{t} \\ \mathbf{s}_2 \cdot \mathbf{e}_1 & \mathbf{s}_2 \cdot \mathbf{e}_2 & \mathbf{s}_2 \cdot \mathbf{t} \\ \mathbf{t} \cdot \mathbf{e}_1 & \mathbf{t} \cdot \mathbf{e}_2 & \mathbf{t} \cdot \mathbf{t} \end{bmatrix} = \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The relationship between $\mathbf{K}_X$ and $\mathbf{K}_S$ is given by

$$\mathbf{K}_X = \mathbf{Q} \mathbf{K}_S \mathbf{Q}^T$$

where $\mathbf{Q}$ is the rotation matrix:

$$\mathbf{Q} = \begin{bmatrix} \mathbf{x} \cdot \mathbf{s}_1 & \mathbf{x} \cdot \mathbf{s}_2 & \mathbf{x} \cdot \mathbf{t} \\ \mathbf{y} \cdot \mathbf{s}_1 & \mathbf{y} \cdot \mathbf{s}_2 & \mathbf{y} \cdot \mathbf{t} \\ \mathbf{z} \cdot \mathbf{s}_1 & \mathbf{z} \cdot \mathbf{s}_2 & \mathbf{z} \cdot \mathbf{t} \end{bmatrix}$$

In 2D, one of the principal curvature directions is always known, so it is possible to define $\mathbf{s}_1$ and $\mathbf{s}_2$ so that they coincide with $\mathbf{e}_1$ and $\mathbf{e}_2$. The rotation matrix $\mathbf{Q}_0$ is the identity, and the auxiliary dependent variable for the angle $\phi$ can be omitted.

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### DERIVATIVES OF THE CURVATURE TENSOR

Following Ref. 13, the derivative of the curvature tensor along the ray trajectory in a graded medium is given by the expression

$$\frac{d\mathbf{K}_S}{ds} = \sum_{i=1}^{5} \mathbf{M}_i$$

where the terms $\mathbf{M}_i$ correspond to the different ways in which the curvature can depend on the medium properties. They are defined using the following expressions:

$$\mathbf{M}_1 = \mathbf{K}_S \cdot \mathbf{K}_S$$

$$\mathbf{M}_2 = -\frac{1}{n}(\mathbf{t} \cdot \nabla_S n)\mathbf{K}_S$$

$$\mathbf{M}_3 = -\frac{1}{n}\Pi(\nabla_S \otimes \nabla_S n)$$

$$\mathbf{M}_4 = \frac{2}{n^2}\Pi(\nabla_S n \otimes \nabla_S n)\Pi$$

$$\mathbf{M}_5 = -\frac{1}{n}[(\mathbf{K}\nabla_S n) \otimes \mathbf{t} + \mathbf{t} \otimes \nabla_S n \mathbf{K}]$$

where $\Pi$ is the projection matrix:

$$\Pi = \mathbf{I} - (\mathbf{t} \otimes \mathbf{t})$$

The gradient operator $\nabla_S$ consists of derivatives that are taken with respect to the local coordinates with basis vectors $\mathbf{s}_1$, $\mathbf{s}_2$, and $\mathbf{t}$.

### DERIVATIVES OF THE PRINCIPAL CURVATURES

By application of the chain rule, the derivatives of the nonzero elements of $\mathbf{K}_S$ can be expressed in terms of the principal curvatures that occupy the diagonal elements of $\mathbf{K}_W$ and the rotation angle $\phi$:

$$\frac{\partial \kappa_1}{\partial s} = \frac{\partial K_{S,11}}{\partial s}\cos^2\phi - 2\frac{\partial K_{S,12}}{\partial s}\sin\phi\cos\phi + \frac{\partial K_{S,22}}{\partial s}\sin^2\phi$$

$$\frac{\partial \kappa_2}{\partial s} = \frac{\partial K_{S,11}}{\partial s}\sin^2\phi + 2\frac{\partial K_{S,12}}{\partial s}\sin\phi\cos\phi + \frac{\partial K_{S,22}}{\partial s}\cos^2\phi$$

$$\frac{\partial \phi}{\partial s} = \frac{1}{\kappa_2 - \kappa_1}\left[\frac{\partial K_{S,12}}{\partial s}\cos(2\phi) + \frac{1}{2}\left(\frac{\partial K_{S,11}}{\partial s} - \frac{\partial K_{S,22}}{\partial s}\right)\sin(2\phi)\right]$$

### NUMERICAL STABILIZATION

The principal curvatures $\kappa_1$ and $\kappa_2$ are not ideal choices for the auxiliary dependent variables stored by each ray because their values can become arbitrarily large as rays approach caustics. Similarly, the principal radii of curvature $r_1$ and $r_2$ are not ideal

choices because their values can become arbitrarily large when a diverging wavefront begins to converge while propagating through a graded medium.

Instead, the auxiliary dependent variables stored by each ray are the help variables $\alpha_1$ and $\alpha_2$. In 2D, only one help variable is allocated because the out-of-plane principal radius of curvature is assumed to be infinite. The principal curvatures are expressed in terms of the help variables using the expression

$$\kappa_i = \kappa_0 \tan \alpha$$

where $\kappa_0 = 1 \; 1/\text{m}$ and $i \in [1, 2]$. The derivatives are then related by the expression

$$\frac{d\alpha_i}{ds} = \frac{1}{\kappa_0}\frac{d\kappa_i}{ds}\cos^2\alpha_i$$

Similarly, the intensity may become infinitely large at caustics, and its reciprocal becomes infinitely large as rays undergo attenuation, so a help variable $\Gamma$ is used to represent the intensity of the ray:

$$I = I_0 \tan \Gamma$$

where $I_0 = 1 \; \text{W/m}^2$. The relationship between the ray intensity help variable and the principal curvatures is

$$\frac{d\Gamma}{ds} = \frac{1}{2}\sin(2\Gamma)[\kappa_1 + \kappa_2 - 2\kappa k_0]$$

where $k_0$ is the free space wave number and $\kappa$ is the imaginary part of the refractive index. Three additional auxiliary dependent variables are used to store information about the remaining Stokes parameters.

## Refraction in Strongly Absorbing Media

The direction of ray propagation may be described via the loci of points having constant phase or amplitude. In a nonabsorbing medium, one which may be described by a real-valued refractive index, changes in the ray intensity are caused only by the convergence or divergence of the wavefront, so the surfaces in which the phase is constant are parallel to the surfaces in which the amplitude is constant.

In a weakly absorbing medium, in which the attenuation of the power transmitted by each ray decays over a length scale much larger than the wavelength, it may be assumed that the surfaces of constant amplitude are still parallel to the surfaces of constant

phase. The directions of the reflected and refracted rays at material discontinuities, as well as the Fresnel coefficients that govern their intensity, may be computed using the real parts of the refractive indices on either side of the boundary. However, as the imaginary part of the refractive index increases in magnitude, this assumption may begin to present a considerable source of error because the surfaces of constant amplitude and surfaces of constant phase are no longer parallel.

In the Settings window for the Geometrical Optics interface, select the **Use corrections for strongly absorbing media** check box in the physics interface **Intensity Computation** section to modify Snell's law and the Fresnel equations to accurately model refraction between media with complex refractive indices. This check box is available when **Intensity computation** is set to **Compute intensity** or **Compute intensity and power**.

Following Chang and others in Ref. 14, the wave vector in an absorbing medium is treated as a bivector with complex components,

$$\mathbf{k} = k_0(N\mathbf{e} - iK\mathbf{f})$$

where $\mathbf{k}$ is the wave vector, $k_0$ is the wave number in free space, and $\mathbf{e}$ and $\mathbf{f}$ are unit vectors with real-valued components indicating the normal direction to the surfaces of constant phase and surfaces of constant amplitude, respectively. The real-valued quantities $N$ and $K$, sometimes called the apparent refractive indices, are related to the complex refractive index by the relations

$$N^2 - K^2 = n^2 - \kappa^2$$

$$NK\mathbf{e} \cdot \mathbf{f} = n\kappa$$

where $n - i\kappa$ is the complex refractive index of the medium. From these relations the apparent refractive indices can be computed as long as the dot product $\mathbf{e} \cdot \mathbf{f}$ is known. To store information about the value of this dot product, auxiliary dependent variables for the components of $\mathbf{f}$ are stored when the **Use corrections for strongly absorbing media** check box is selected.

At material discontinuities, the normal vectors to the surfaces of constant amplitude and phase follow a modified form of Snell's law that uses the apparent refractive indices,

$$N_1 \sin\theta_1 = N_2 \sin\theta_2$$

$$K_1 \sin\Psi_1 = K_2 \sin\psi_2$$

where $\theta$ and $\psi$ are the acute angles between the surface normal and the normal vectors to the surfaces of constant phase and surfaces of constant amplitude, respectively. The real part of the apparent refractive index in the second domain is a root of the quartic equation

$$AN_2^4 + BN_2^2 + C = 0$$

$$
\begin{aligned}
A &= 1 \\
B &= -[N_s^2 + K_s^2 + (n_2^2 - \kappa_2^2)] \\
C &= N_s^2 K_s^2 + (n_2^2 - \kappa_2^2)N_2^2 - (nk - N_s K_s \cos\phi)^2
\end{aligned}
$$

where $N_s = N_1 \sin\theta_1$, $K_s = K_1 \sin\psi_1$, and the angle $\phi$ is the azimuthal angle between the normal to surfaces of constant amplitude and the plane of incidence. This equation is obviously quadratic in $N_2^2$ and can thus be solved using the quadratic formula.

The reinitialized unit normal vectors to the surfaces of constant amplitude and phase are

$$\mathbf{e}_2 = \frac{N_1}{N_2}\mathbf{e}_1 + \left(\cos\theta_2 - \frac{N_1}{N_2}\cos\theta_1\right)\mathbf{n}$$

$$\mathbf{f}_2 = \frac{K_1}{K_2}\mathbf{f}_1 + \left(\cos\psi_2 - \frac{K_1}{K_2}\cos\psi_1\right)\mathbf{n}$$

whereas for the reflected ray the reinitialized unit normal vectors are

$$\mathbf{e}_2 = \mathbf{e}_1 - 2\mathbf{n}\cos\theta$$

$$\mathbf{f}_2 = \mathbf{f}_1 - 2\mathbf{n}\cos\psi$$

## Attenuation Within Domains

Rays can gradually lose energy as they propagate through a domain in which the refractive index is complex. The convention of the Geometrical Optics interface is that a lossy medium has refractive index given by $n - i\kappa$. Given the electric field $\mathbf{E}_0$ at one location, the electric field of a ray with infinite wavefront radii of curvature as it propagates through a homogeneous, lossy medium is

$$|\mathbf{E}| = |\mathbf{E}_0| \exp\left(-\frac{k_0 KL}{N}\cos\alpha\right)$$

where $L$ is the optical path length between the points at which $\mathbf{E}$ and $\mathbf{E}_0$ are measured and $k_0$ is the wave number in free space. In weakly absorbing media, $N = n$, $K = \kappa$, and $\alpha = 0$. If the **Use corrections for strongly absorbing media** check box is selected, $N$ is the real part of the apparent refractive index, $K$ is the complex part of the apparent refractive index, and $\alpha$ is the angle between the surfaces of constant amplitude and surfaces of constant phase; both of these concepts are explained in Refraction in Strongly Absorbing Media. The ray intensity and power are both proportional to the square of the electric field norm, so these quantities change according to the relations

$$I = I_0 \exp\left(-\frac{2k_0 KL}{N}\cos\alpha\right)$$

$$P = P_0 \exp\left(-\frac{2k_0 KL}{N}\cos\alpha\right)$$

When computing the ray intensity in absorbing media, the principal radii of curvature of the wavefront must also be considered. The two contributing factors are accounted for by allocating auxiliary dependent variables for the initial Stokes parameters following the most recent reinitialization of the wave vector, which are expressed as solutions to first-order differential equations of the form

$$\frac{ds_{i,0}}{dt} = -2k_0 Kcs_{i,0} \qquad i \in \{0, 1, 2, 3\} \tag{3-20}$$

where $c$ is the speed of light in the medium and $s_{i,0}$ is value of one of the Stokes parameters of the ray before the effects of changes in the principal radii of curvature have been applied.

The Geometrical Optics interface defines an additional dependent variable $A$ (dimensionless) for the path integral of the attenuation coefficient,

$$\frac{dI_0}{dt} = 0 \tag{3-21}$$

$$I = I_0 \exp(A)$$

$$\frac{dA}{dt} = -2k_0 Kc$$

Despite requiring an extra degree of freedom per ray, the advantage of Equation 3-21 over Equation 3-20 is that the dependent variables in Equation 3-21 all vary linearly within a homogeneous medium. This makes Equation 3-21 less prone to numerical stiffness; it remains more accurate when the solver takes long time steps, compared to Equation 3-20, potentially reducing solution time and improving accuracy.

*Fluence Rate Calculation Theory*

The fluence rate $E_0$ (SI unit: W/m$^2$) is a volume quantity that indicates potential exposure to radiation. The fluence rate at any point in a domain is the total incident power that would hit a small spherical target at that location, from all directions, divided by the cross sectional area of the sphere (Ref. 16).

For the purpose of defining fluence rate the "small sphere" is an opaque detector whose radius is much smaller than any geometry details in the model, but substantially larger than the wavelength of radiation. Thus, the absorption cross section of the sphere is equal to its geometrical cross section and it is not necessary to consider Mie scattering theory.

In the path of a collimated beam of uniform intensity $I$ (SI unit: W/m$^2$), the fluence rate is simply $I$; however, the fluence rate distribution may be more complicated if there are multiple beams intersecting at a point (since fluence rate takes contributions from radiation arriving in all directions), or if the radiation is diffusely emitted or reflected.

The Fluence Rate Calculation node is a special type of Accumulator (Domain) that can be added to a model when the ray power is solved for, meaning that one of the options **Compute power**, **Compute intensity and power**, or **Compute intensity and power** in graded media should be selected from the physics interface **Intensity Computation** list. This feature defines an accumulated variable in each domain mesh element that gets the following contribution from rays as they propagate through the element:

$$\frac{\partial E_0}{\partial t} = \frac{1}{\text{meshvol}}\sum_i Q_i c_i$$

where the sum is taken over the rays within each mesh element, $Q_i$ (SI unit: W) is the ray power, and $c_i$ (SI unit: m/s) is the speed of light of the ray. The division by the mesh element volume **meshvol** compensates for the tendency of a larger domain element to intersect a greater number of rays. Rather than a time integral, the above can be thought of as a path integral of ray power from the entrance point to the exit point as each ray traverses the mesh element.

The key distinction between fluence rate and deposited power is that fluence rate can be nonzero even if the medium is not absorbing; it represents the potential for a small object to be irradiated even if that object can only block a tiny fraction of the radiation in the domain.

## Ray Termination Theory

The Ray Termination feature can annihilate rays when their intensity or power decreases below a specified threshold.

If the ray intensity is computed, then the threshold ray intensity $I_{th}$ (SI unit: $W/m^2$) can be specified. Then the termination criterion is

$$I < I_{th}$$

If the ray power is computed, then the threshold ray power $Q_{th}$ (SI unit: W) can be specified. Then the termination criterion is

$$Q < Q_{th}$$

It is also possible to specify termination criteria based on both intensity and power; in this case, the rays terminate if either criterion is satisfied.

Whenever possible, the **Ray Termination** feature attempts to stop rays at the exact instant when the ray intensity or power reaches a specified threshold value. A closed-form analytic solution for the exact stop time is available under the following circumstances:

- The rays represent planar wavefronts in an absorbing medium, or
- The rays represent spherical or ellipsoidal wavefronts in a nonabsorbing medium.

If neither of these special conditions is met, the ray can only terminate if the termination criterion is met at the beginning of a time step taken by the solver; the ray intensity or power at the instant the ray is stopped may be less than the threshold.

### PLANAR WAVEFRONTS IN AN ABSORBING MEDIUM

In this special case, the principal wavefront radii of curvature are so large that the ray intensity can only change significantly in an attenuating medium. The exact time $t_s$ (SI unit: s) at which the ray intensity reaches the threshold value is

$$t_s = t_0 + \tau \log\left(\frac{I}{I_{th}}\right)$$

where

- $t_0$ (SI unit: s) is the previous time step, reflection time, or refraction time,
- $I$ (SI unit: $W/m^2$) is the intensity at $t_0$, and
- $I_{th}$ (SI unit: $W/m^2$) is the threshold intensity.

If the termination criterion is based on the ray power $Q$ (SI unit: W) instead of ray intensity, the analogous expression for the stop time is

$$t_s = t_0 + \tau \log\left(\frac{Q}{Q_{th}}\right)$$

The characteristic time for ray attenuation $\tau$ (SI unit: s) is

$$\tau = \frac{\lambda_0 N}{4\pi c K}$$

where

- $\lambda_0$ (SI unit: m) is the free-space wavelength of the radiation,
- $N - iK$ (dimensionless) is the apparent refractive index of the medium, where $N$ and $K$ are real numbers, and
- $c = 299{,}792{,}458$ m/s is the speed of light in a vacuum.

### DIVERGING WAVEFRONTS IN A NONABSORBING MEDIUM

In a nonabsorbing medium in which the wavefront is nonplanar, the ray can only terminate due to the intensity decreasing below the threshold, since the power does not change. The time $t_s$ (SI unit: s) at which the ray intensity reaches the threshold in a nonattenuating, homogeneous medium is

$$t_s = t_0 + \frac{1}{2V_g}\left(r_1 + r_2 + \sqrt{(r_1 - r_2)^2 + 4\frac{I}{I_{th}}|r_1 r_2|}\right)$$

where

- $t_0$ (SI unit: s) is the previous time step, reflection time, or refraction time,
- $V_g$ (SI unit: m/s) is the group velocity magnitude,
- $r_1$ (SI unit: m) is the first principal radius of curvature of the wavefront at $t_0$,
- $r_2$ (SI unit: m) is the second principal radius of curvature of the wavefront at $t_0$,
- $I$ (SI unit: W/m$^2$) is the intensity at $t_0$, and
- $I_{th}$ (SI unit: W/m$^2$) is the threshold intensity.

In 2D models, or in 3D models where the wavefronts are cylindrical (one extremely large radius of curvature and one finite radius of curvature), the stop time is instead

$$t_s = t_0 + \frac{1}{V_g}\left(r_1 + \frac{I}{I_{th}}|r_1|\right)$$

where $r_1$ (SI unit: m) is the finite principal radius of curvature of the cylindrical wavefront.

## Illuminated Surface Theory

The Illuminated Surface is used to simulate the emission of rays from a surface, under the assumption that the emitted rays are specularly reflected from an external radiation source. It is assumed that the entire selected surface has direct line of sight to the external radiation source; that is, shadowing due to other geometric entities is not taken into account.

If the Incident ray direction vector is a **User defined direction** or based on **Solar position**, the incident rays are treated as plane waves arriving from a distant source, and the intensity of the incident rays $I_i$ is specified directly.

If the **Incident ray direction vector** is computed using a **User defined point source**, the principal radii of curvature of the incident wavefront are set equal to the distance from the source point to the initial ray position,

$$r_1 = r_2 = -\left|\mathbf{r}_{src} - \mathbf{q}\right|$$

where $\mathbf{q}$ is the initial ray position, $\mathbf{r}_{src}$ is the position vector of the point source, and $r_1$ and $r_2$ are the principal radii of curvature of the incident wavefront. In 2D, only one principal radius of curvature is defined. The incident ray intensity is derived from the total source power $P_{src}$,

$$I_i = \frac{P_{src}}{4\pi\left|\mathbf{r}_{src} - \mathbf{q}\right|}$$

The principal radii of curvature of the reflected rays are then computed using the approach outlined in the Principal Radii of Curvature section. Because no thin films are present on the surface, the intensity of the reflected ray is equal to the intensity of the incident ray. The effect of specular reflection is to negate the third and fourth Stokes parameters of the ray.

**ANGULAR PERTURBATIONS**

It is often necessary to take the finite size of a radiation source into account when modeling the reflection or refraction of rays at an illuminated surface. This is particularly true in solar energy applications, in which the finite size of the solar disk significantly affects the focusing capability of solar concentrating devices.

To release rays with a distribution of initial directions based on the finite size of the radiation source, select **Create light cones at release points** or **Sample from conical distribution** option from the **Corrections for finite source diameter** check box in the settings window for the Illuminated Surface feature.

Selecting **Create light cones at release points** causes a cone of rays to be released at each release point. Selecting **Sample from conical distribution** causes only a single ray to be released at each point, but each ray's initial direction is sampled form a cone-shaped probability distribution function. The maximum angle between any incident ray and the specified incident ray direction is the user-defined maximum disk angle $\psi_m$ (SI unit: rad).

The options described above are also available in the settings window for the Solar Radiation feature, in which they have the same effects on the initial direction of the solar radiation.

*Limb Darkening*
The default value of the maximum disk angle, or the maximum angle between the direction of the incident rays and the specified **Incident ray direction vector**, is $\psi_m = 4.65$ mrad based on the following expressions (see for example Ref. 22):

$$\psi_m = \text{asin}\left(\frac{d_{sun}}{2L_0}\right)$$

$$d_{sun} = 1.392 \times 10^9 \, m$$

$$L_0 = 1.496 \times 10^{11} \, m$$

When the finite size of the sun is taken into account, radiation from the center of the solar disc tends to be greater in intensity than radiation from the edges of the disc, a phenomenon known as limb darkening. If **Empirical power law** is selected from the **Limb darkening model** list in the settings window for the **Illuminated Surface** or **Solar Radiation** feature, the solar radiation is assumed to follow a power law distribution. Given the intensity $I(0)$ of radiation along a line intersecting the center of the sun, the incident solar radiation from any other point on the sun is given by the expression

$$\frac{I(\psi_s)}{I(0)} = \mu^{\alpha(\lambda_0)}$$

where

$$\mu = \cos\psi_s$$

and $\psi_s$ is the angle between a line of sight to the center of the sun and a line from the center of the sun to another visible point on its surface. The exponent $\alpha$ can vary from 0, for which all solar radiation is of uniform intensity, to 1, at which the intensity of solar radiation falls off linearly as a function of radial position on the visible solar disc. Based on Ref. 22 the exponent $\alpha$ is given as a function of the free-space wavelength $\lambda_0$:

$$
\alpha(\lambda_0) = \begin{cases} -0.023 + 0.292\lambda_0^{-1} & \lambda_0^{-1} \leq 2.4\mu\mathrm{m}^{-1} \\ 0.3778 + 0.125\lambda_0^{-1} & 2.4\mu\mathrm{m}^{-1} \leq \lambda_0^{-1} \leq 2.8\mu\mathrm{m}^{-1} \\ -0.507 + 0.441\lambda_0^{-1} & 2.8\mu\mathrm{m}^{-1} \leq \lambda_0^{-1} \end{cases}
$$

If **Linear** is selected from the **Limb darkening model** list, the distribution of solar intensity is instead

$$
\frac{I(\psi_s)}{I(0)} = \frac{1 + \beta\mu}{1 + \beta}
$$

*Surface Roughness*

It is also possible to include the effect of surface roughness when computing the incident ray direction vector at illuminated surfaces by selecting the **Include surface roughness** check box. The value of the **Surface slope error** $\sigma$ is used as the standard deviation in a Rayleigh distribution of perturbation angles about the unperturbed ray direction vector, from which a user-defined number of rays are sampled. For more details see Surface Slope Error.

## *Theory of Mueller Matrices and Optical Components*

Optical devices such as polarizers and wave retarders are often used to manipulate the polarization of radiation. These devices can be modeled by multiplying the Stokes vector of the incident ray $\mathbf{s_i}$ by a Mueller matrix $\mathbf{M}$,

$$
\mathbf{s} = \mathbf{M}\mathbf{s_i}
$$

As explained in The Stokes Parameters, the Stokes vector requires a set of orthogonal coordinate axes to be defined at the location of a propagating ray. The $x$-axis of this local coordinate system, $\mathbf{e_1}$, is the first principal curvature direction in 3D models and the out-of-plane direction in 2D models.

Similarly, the Mueller matrix of an optical device is defined with respect to a local coordinate system. This system need not coincide with the coordinate system that defines the Stokes vector of the incident ray. Therefore it is usually necessary to apply a rotation to one of these local coordinate systems before applying the Mueller matrix:

$$\mathbf{s} = \mathbf{R}^{-1}\mathbf{M}\mathbf{R}\mathbf{s}_i$$

where $\mathbf{R}$ is the rotation matrix

$$R = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(2\theta) & \sin(2\theta) & 0 \\ 0 & -\sin(2\theta) & \cos(2\theta) & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

where $\theta$ is the angle by which the local coordinate system of the ray must be rotated so that the $x$-axes of the two local coordinate systems both lie in the plane of incidence and the $y$-axes are parallel.

Mueller matrices of some common optical devices are tabulated in Ref. 15.

### LINEAR POLARIZER THEORY

A Linear Polarizer is an optical device that produces linearly polarized light. An ideal linear polarizer transmits radiation that is polarized in one direction, indicated by the transmission axis $\mathbf{T}$, while completely preventing the transmission of radiation polarized in the orthogonal direction.

In a local coordinate system in which the $x$-axis is parallel to the transmission axis, the Mueller matrix of the ideal linear polarizer is

$$\mathbf{M} = \frac{1}{2}\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

### LINEAR WAVE RETARDER THEORY

A Linear Wave Retarder is an optical device that separates a ray into two rays with orthogonal linear polarizations, retards the phase of one of these rays with respect to the other, and then recombines the two rays. The direction of polarization that undergoes this retardation is called the slow axis, and the orthogonal direction is called

the fast axis **F**. The phase delay between the two orthogonal components is the retardance $\delta$ of the device.

In a local coordinate system in which the $x$-axis is parallel to the fast axis, the Mueller matrix of an ideal linear wave retarder is

$$\mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \cos\delta & \sin\delta \\ 0 & 0 & -\sin\delta & \cos\delta \end{bmatrix}$$

For example, a quarter-wave retarder ($\delta = \pi/2$) converts circularly polarized light to linearly polarized light, whereas a half-wave retarder ($\delta = \pi$) converts left-handed circularly polarized light to right-handed circularly polarized light.

### CIRCULAR WAVE RETARDER THEORY

A Circular Wave Retarder, or polarization rotator, is an optical device that separates a ray into two rays with left-handed and right-handed circular polarizations, retards the phase of one of these rays with respect to the other, and recombines the two rays. A right circular polarization rotator is represented by the Mueller matrix

$$\mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\delta & \sin\delta & 0 \\ 0 & -\sin\delta & \cos\delta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

The circular retarder rotates the polarization ellipse of the incident ray by an angle $\delta/2$ about the origin.

### IDEAL DEPOLARIZER THEORY

The Ideal Depolarizer converts radiation of any polarization to completely unpolarized radiation. The Mueller matrix of an ideal depolarizer is

$$\mathbf{M} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

## *Thin Dielectric Film Theory*

When ray intensity or power is solved for, thin dielectric films can be used to change the reflection and transmission coefficients at boundaries. Individual dielectric layers can be applied to a boundary by using the Thin Dielectric Film subnode, which can be added to the Material Discontinuity and Wall nodes. The **Thin Dielectric Film** subnode can be added to the same boundary multiple times to create multilayer films. In general, the thickness of these thin dielectric films is comparable in magnitude to the wavelength of the rays; a minimum requirement is that the thickness of each layer is much less than the coherence length of the incident rays.

### COMPUTING THE FRESNEL COEFFICIENTS OF BOUNDARIES WITH THIN DIELECTRIC FILMS

When the **Thin Dielectric Film** feature is used to model dielectric layers, the equivalent Fresnel coefficients for ray propagation through the layer are computed using a recursive algorithm. These equivalent Fresnel coefficients are, in general, complex-valued reflection and transmission coefficients that account for the phase delay and amplitude change in the reflected and transmitted rays resulting from the multiple reflections that the ray undergoes within the dielectric layer, all of which are considered to be coherent with each other. As these multiple reflected and refracted rays propagate into the domains adjacent to the film, they can interfere constructively or destructively with each other, which affects the total electric field amplitude that propagates into each domain. This is illustrated in Figure 3-13 below. Due to the rays' capability to interfere constructively or destructively with each other, the optical thickness of the thin film has a significant effect on the amplitude and phase of the reflected and refracted rays.
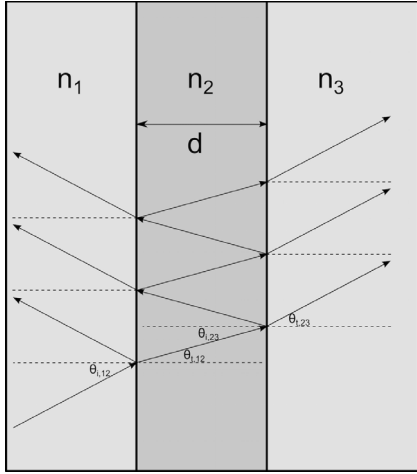
*Figure 3-13: One incident ray enters a thin dielectric film and produces a large number of coherent reflected and refracted rays in the adjacent semi-infinite media. These rays can interfere constructively or destructively with each other.*

Consider, as shown above, a thin film of thickness $d$ and refractive index $n_2$ bounded by semi-infinite domains with refractive indices $n_1$ and $n_3$. Also consider a linearly polarized ray with electric field amplitude $E_0$ that propagates through the domain of refractive index $n_1$ and interacts with the thin film. Let the coefficients of refraction and transmission for a ray moving from the domain of refractive index $n_a$ to the domain of refractive index $n_b$ be denoted $r_{ab}$ and $t_{ab}$, respectively. When the ray arrives at the film, the refracted ray undergoes a series of reflections at the boundaries between the film and either adjacent domain. Following Ref. 9, the amplitudes of the refracted rays in either domain form a pair of converging geometric series with sums

$$r_{eq} = \frac{E_1}{E_0} = r_{12} + t_{12}t_{21}r_{23}e^{2i\beta} \sum_{k=0}^{\infty} (r_{21}r_{23}e^{2i\beta})^k = \frac{r_{12} + r_{23}e^{2i\beta}}{1 + r_{12}r_{23}e^{2i\beta}}$$

for rays returning to the domain of refractive index $n_1$, and

$$t_{eq} = \frac{E_3}{E_0} = t_{12}t_{23}e^{i\beta} \sum_{k=0}^{\infty} (r_{21}r_{23}e^{2i\beta})^k = \frac{t_{12}t_{23}e^{i\beta}}{1 + r_{12}r_{23}e^{2i\beta}}$$

for rays entering the domain of refractive index $n_3$. The angle $\beta$ is the phase delay that is introduced when a ray propagates from one surface of the film to the other,

$$\beta = \frac{2\pi n_2 d \cos\theta_2}{\lambda_0} \tag{3-22}$$

where $\lambda_0$ is the free-space wavelength and $\theta_2$ is the angle between the wave vector of a ray within the thin film and the normal to the film. The dielectric film can be modeled as a material discontinuity with transmission and reflection coefficients $t_{eq} = E_3 / E_0$ and $r_{eq} = E_1 / E_0$.

> Several derivations for the equivalent Fresnel coefficients are also given by Heavens in Ref. 17, including recursive algorithms and matrix formulations. However, the sign conventions and symbols used in this section have been selected to be consistent with Born and Wolf (Ref. 9) and therefore differ from those in Ref. 17.

### AUTOMATIC SETUP OF SINGLE-LAYER FILMS

The Material Discontinuity node includes options for automatic setup of single-layer films with specified reflectance $R$ or transmittance $T$. In either case the layers are assumed to be nonabsorbing, so that $R + T = 1$. To enable these options, select **Specify reflectance** or **Specify transmittance** from the **Thin dielectric films on boundary** list, and then select the **Treat as single layer dielectric film** check box.

The specified reflectance $R$ of a thin film with refractive index $n$ is valid only for certain values of the angle of incidence $\theta_i$ and free-space wavelength $\lambda_0$. After computing the Fresnel coefficients for rays entering and leaving the layer, the reflectance can be expressed as

$$R = \left| \frac{r_{12} + r_{23}e^{2i\beta}}{1 + r_{12}r_{23}e^{2i\beta}} \right|^2 = \frac{r_{12}^2 + r_{23}^2 + 2r_{12}r_{23}\cos(2\beta)}{r_{12}^2 r_{23}^2 + 2r_{12}r_{23}\cos(2\beta) + 1}$$

Solving this expression for $\beta$ and substituting the result into Equation 3-22 yields

$$d = \left| \frac{\lambda_0}{4\pi n \cos\theta_2} \mathrm{acos}\left( \frac{r_{12}^2 r_{23}^2 R - r_{12}^2 - r_{23}^2 + R}{2r_{12}^2 r_{23}^2 (1 - R)} \right) \right|$$

For nonzero angles of incidence, the layer thickness that yields a specified reflectance or transmittance depends on the ray polarization. The coefficients of reflection for rays

propagating into or out of the layer are either those for S- or P-polarized radiation, depending on the selected option in the **Specified film behavior applies to** list.

> ⚠️ In some cases, the specified transmittance or reflectance will be impossible to achieve, given the refractive indices of the layer and the surrounding media. In such cases, rays will pass through the boundary as if no dielectric layers were present.

### AUTOMATIC SETUP OF ANTI-REFLECTIVE COATINGS

To automatically compute the refractive index and thickness of a single-layer anti-reflective coating between two dielectric media, in the settings for the Material Discontinuity node select **Anti-reflective coating** from the **Thin dielectric films on boundary** list. By default the anti-reflective coating is ideal, in the sense that is always has a reflectance of zero for rays of any wavelength and any angle of incidence. However, if you select the **Treat as single layer dielectric film** check box, then instead the single-layer coating only has a reflectance of zero for rays at a specific angle of incidence $\theta_i$ (SI unit: rad) and vacuum wavelength $\lambda_0$ (SI unit: m).

For oblique incidence, the refractive index of the ideal single-layer coating differs for $s$- and $p$-polarized rays. For $s$-polarized rays, the refractive index $n_2$ of a film between media with refractive indices $n_1$ and $n_3$ is

$$n_2 = \sqrt{(n_1 \sin\theta_i)^2 + n_1\cos\theta_i\sqrt{n_3^2 - (n_1\sin\theta_i)^2}}$$

For $p$-polarized rays, the refractive index is

$$n_2 = \frac{\sqrt{2}}{2}\frac{\sqrt{\cos\theta_i n_a n_1 (n_3 + \sqrt{n_3^2 - 4\cos\theta_i\sin^2\theta_i n_a n_1 n_3})}}{n_a\cos\theta_i}$$

where

$$n_a \equiv \frac{n_3^2 - (n_1\sin\theta_i)^2}{n_3^2}$$

Either equation returns the value of $n_2$ for which $r_{12} = r_{23}$ for rays of the specified polarization at the specified angle of incidence. An ideal anti-reflective coating is obtained when the magnitude of the equivalent reflection coefficient is 0. This can be

obtained when $r_{12} = r_{23}$ and the phase delay $\delta$ is equal to $\pi/2$. Substituting this requirement into Equation 3-22 yields an expression for $d$:

$$d = \frac{\lambda_0}{4 n_2 \cos \theta_2}$$

### SETUP OF REPEATING MULTILAYER FILMS

It is possible to identify a unit cell consisting of a small number of thin dielectric films and to repeat these layers a specified number of times. To set up repeating multilayer films, select **Add layers to surface, repeating** from the **Thin dielectric films on boundary** list.

Select the **Repeat layer in multilayer films** check box in the **Repeating Multilayer Films** section of the Thin Dielectric Film settings window to include the layer in the unit cell of a repeating multilayer film. It is possible to include some layers in the unit cell while excluding others. This could be used, for example, to ensure that a repeating multilayer film begins and ends with the same layer, since in this case the last layer is not included in any unit cell. However, the **Thin Dielectric Film** nodes for all layers in the unit cell must be adjacent to each other in the Model Builder.

Enter a value or expression for the **Number of repeating unit cells** $N$ in the Material Discontinuity settings window. If there are $p$ **Thin Dielectric Film** nodes in which the **Repeat layer in multilayer films** check box is selected and $q$ **Thin Dielectric Film** nodes in which the **Repeat layer in multilayer films** check box is cleared, the total number of dielectric layers in the multilayer film $N_t$ will be $Np + q$.

The recursive algorithm described in the section Computing the Fresnel Coefficients of Boundaries with Thin Dielectric Films is not well-suited to the calculation of the effective Fresnel coefficients for an extremely large number of thin dielectric films in a periodic arrangement. Instead, the following approach is used, in which the equivalent Fresnel coefficients are expressed in terms of the product of a large number of 2-by-2 matrices.

Let the electric field amplitude of the incident, reflected, and transmitted rays entering layer $m$ be denoted $E_m^i$, $E_m^r$, and $E_{m+1}^i$, respectively, where $m \in [1, N_t]$. The ratios of the incoming and outgoing electric field amplitudes in consecutive layers $m$ and $m+1$ are

$$\begin{bmatrix} E_m^i \\ E_m^r \end{bmatrix} = \frac{1}{t_{(m-1)(m)}} \mathbf{C}_m \begin{bmatrix} E_{m+1}^i \\ E_{m+1}^r \end{bmatrix}$$

Where $\mathbf{C}_m$ is a 2-by-2 matrix:

$$\mathbf{C}_m = \begin{bmatrix} C_{m,11} & C_{m,12} \\ C_{m,21} & C_{m,22} \end{bmatrix} = \begin{bmatrix} \exp(-i\delta_{m-1}) & r_{(m-1)(m)}\exp(-i\delta_{m-1}) \\ r_{(m-1)(m)}\exp(i\delta_{m-1}) & \exp(i\delta_{m-1}) \end{bmatrix}$$

where $\delta_{m-1}$ is the phase shift within the layer, with $\delta_0 = 0$.

For a multilayer film containing $N_t$ layers including $N$ unit cells, the relationship between the incoming and outgoing electric field amplitudes can be expressed using the product of $N_t + 1$ matrices and $N_t + 1$ transmission coefficients:

$$\begin{bmatrix} E_0^i \\ E_0^r \end{bmatrix} = \left( \prod_{m=1}^{N_t+1} t_{(m-1)(m)} \right)^{-1} \left( \prod_{m=1}^{N_t+1} \mathbf{C}_m \right) \begin{bmatrix} E_{N_t+1}^i \\ E_{N_t+1}^r \end{bmatrix}$$

To simplify the matrix multiplication, the product of the matrices can be expressed in the form

$$\prod_{m=1}^{N_t+1} \mathbf{C}_m = \mathbf{C}_{in}(\mathbf{C}_{cell})^N \mathbf{C}_{out}$$

where $\mathbf{C}_{in}$ is the product of the matrices for all layers prior to the unit cell, $\mathbf{C}_{out}$ is the product of the matrices for all layers following the unit cell, and $\mathbf{C}_{cell}$ is the matrix for all layers within one unit cell, including the interface between one unit cell and the next. Next an eigenvalue decomposition is performed on $\mathbf{C}_{cell}$:

$$\mathbf{C}_{cell} = \mathbf{XDX}^{-1}$$

where $\mathbf{D}$ is a diagonal matrix with nonzero elements $D_{11}$ and $D_{22}$. The ratio of the incoming and outgoing electric field amplitudes can then be expressed as

$$\begin{bmatrix} E_0^i \\ E_0^r \end{bmatrix} = \left( \prod_{m=1}^{N_t+1} t_{(m-1)(m)} \right)^{-1} \mathbf{C}_{in}\mathbf{X} \begin{bmatrix} D_{11}^N & 0 \\ 0 & D_{22}^N \end{bmatrix} \mathbf{X}^{-1}\mathbf{C}_{out} \begin{bmatrix} E_{N_t+1}^i \\ E_{N_t+1}^r \end{bmatrix}$$

Because there is no reflected ray beyond the last dielectric layer, $E_{N_t+1}^r = 0$ and the equivalent Fresnel coefficients of the multilayer film can now be obtained:

$$r_{eq} = \frac{E_0^r}{E_0^i} \qquad t_{eq} = \frac{E_{N_t+1}^i}{E_0^i}$$

## *Diffraction Grating Theory*

The Grating and Cross Grating features are boundary conditions that release rays into one or more diffraction orders whenever a ray hits a boundary. In reality, the grating surface is a periodic substructure in which the unit cells can be smaller than the electromagnetic wavelength, but the substructure geometry is not explicitly modeled as part of the ray optics simulation. Based on the unit cell size and wavelength, rays that hit the grating will propagate into specific directions (the diffraction orders) in which waves from neighboring unit cells would constructively interfere.

Although the substructure of a grating or cross grating may contain many fine details, typically on the micron scale, from a ray optics perspective it is not necessary to explicitly model the substructure geometry. Instead the grating is approximated as a featureless surface where diffraction orders are released in directions computed from the specified unit cell size and the electromagnetic wavelength.

### DEFINITIONS

Unless otherwise stated, in this section, the term "grating" will be used to refer to a surface whose substructure is periodic in one direction and homogeneous in the orthogonal direction. The term "cross grating" will be used for a surface whose substructure exhibits periodicity in two different directions.

Consider an electromagnetic wave incident on the grating or cross grating surface with vacuum wavelength $\lambda_0$ (SI unit: m). It therefore has angular frequency $\omega = 2\pi/\lambda_0$ (SI unit: rad/m). Assuming the surrounding media are transparent or weakly absorbing, the ray propagates in the direction of its wave vector $\mathbf{k}$ (SI unit: rad/m) which has magnitude $k = \omega n/c$. Here $n$ (dimensionless) is the absolute refractive index of the material and $c = 299,792,458$ m/s is the speed of light in a vacuum.

### GRATING

The effect of a grating is to offset the in-plane components of the wave vector by an integer multiple of the reciprocal lattice vector $\mathbf{G}$ (SI unit: rad/m), given by

$$\mathbf{G} = 2\pi\frac{\mathbf{T}_g}{d},$$

Here $d$ (SI unit: m) is the grating constant, that is, the width of each unit cell of the periodic substructure; and $\mathbf{T}_g$ (dimensionless) is a unit vector that lies in the grating surface and indicates the direction of periodicity. By definition, $\mathbf{T}_g$ is orthogonal to the surface normal $\mathbf{n}_s$.

The wave vector $\mathbf{k}$ of the incident ray can be treated as the vector sum of two constituent vectors, one parallel to the surface ($\mathbf{k}_p$) and one perpendicular to it ($\mathbf{k}_n$):

$$\mathbf{k}_p = \mathbf{n}_s \times (\mathbf{k} \times \mathbf{n}_s) \qquad \mathbf{k}_n = (\mathbf{k} \cdot \mathbf{n}_s)\mathbf{n}_s \quad ,$$

The in-plane component of the outgoing wave vector is given by

$$\mathbf{k}_{p,\,out} = \mathbf{k}_p + m\mathbf{G} \tag{3-23}$$

where $m$ (dimensionless) is an integer known as the diffraction order. For $m = 0$ the ray is specularly reflected if it propagates into the same medium as the incident ray, or refracted (as in Snell's law) if it propagates into the medium on the opposite side of the grating. The diffraction order $m$ can be any integer but (as detailed in a later section) rays of a given diffraction order can only propagate if the out-of-plane wave vector component remains real-valued while the in-plane component satisfies Equation 3-23.

### CROSS GRATING

In a **Cross Grating**, the in-plane component of the wave vector is offset by integer multiples of two different reciprocal lattice vectors corresponding to two directions of periodicity in the grating surface,

$$\mathbf{k}_{p,\,out} = \mathbf{k}_p + m\mathbf{G}_1 + n\mathbf{G}_2 \tag{3-24}$$

where $m$ and $n$ are the diffraction order numbers. The two reciprocal lattice vectors $\mathbf{G}_1$ and $\mathbf{G}_2$ (SI unit: rad/m) are defined as

$$\mathbf{G}_1 = 2\pi \frac{\mathbf{d}_2 \times \mathbf{n}_s}{\mathbf{d}_1 \cdot (\mathbf{d}_2 \times \mathbf{n}_s)} \qquad \mathbf{G}_2 = 2\pi \frac{\mathbf{n}_s \times \mathbf{d}_1}{\mathbf{d}_2 \cdot (\mathbf{n}_s \times \mathbf{d}_1)} \tag{3-25}$$

$$\mathbf{d}_1 \equiv d_1 \mathbf{T}_{g,\,1} \qquad \mathbf{d}_2 \equiv d_2 \mathbf{T}_{g,\,2}$$

where $d_1$ and $d_2$ (SI unit: m) are the dimensions of one unit cell in the two-dimensional periodic substructure, and $\mathbf{T}_{g,1}$ and $\mathbf{T}_{g,2}$ (dimensionless) are unit vectors indicating the corresponding directions of periodicity.

Note that $\mathbf{T}_{g,1}$ and $\mathbf{T}_{g,2}$ are not required to be perpendicular to each other, but they cannot be parallel or antiparallel. By definition, both $\mathbf{T}_{g,1}$ and $\mathbf{T}_{g,2}$ are orthogonal to

the surface normal $\mathbf{n}_s$. For the simplified case where $\mathbf{T}_{g,1}$ and $\mathbf{T}_{g,2}$ are perpendicular, Equation 3-25 simplifies to

$$\mathbf{G}_1 \ = \ 2\pi \frac{\mathbf{T}_{g,1}}{d_1} \qquad \mathbf{G}_2 \ = \ 2\pi \frac{\mathbf{T}_{g,2}}{d_2}$$

Similar to a grating with a single direction of periodicity, the two diffraction orders $m$ and $n$ can take on any integer values, but that diffraction order can only propagate if the out-of-plane wave vector component can be real-valued while the in-plane component satisfies Equation 3-24.

### WAVE VECTOR REINITIALIZATION

The magnitude of the outgoing perpendicular component of the reflected and transmitted wavefront can be found from the requirement that the magnitude of the outgoing wave vector $\mathbf{k}_{out}$ is equal to the wave number; that is, $||\mathbf{k}_{out}|| = k_0 n$, where $k_0 = \omega/c$ is the wave number in free space. The projections of the reflected and transmitted wave vectors onto the surface normal $\mathbf{k}_{n,r}$ and $\mathbf{k}_{n,t}$ therefore have magnitudes

$$\begin{aligned}
\|\mathbf{k}_{n,r}\| \ &= \ \sqrt{(k_0 n_1)^2 - \|\mathbf{k}_{p,out}\|^2} \\
\|\mathbf{k}_{n,t}\| \ &= \ \sqrt{(k_0 n_2)^2 - \|\mathbf{k}_{p,out}\|^2}
\end{aligned} \tag{3-26}$$

where $n_1$ and $n_2$ are the refractive indices on the incoming (reflected) and outgoing (transmitted) side of the grating, respectively. The outgoing reflected and transmitted wave vectors $\mathbf{k}_r$ and $\mathbf{k}_t$ are therefore given by

$$\begin{aligned}
\mathbf{k}_r \ &= \ \mathbf{k}_{p,out} + \|\mathbf{k}_{n,r}\| \mathbf{n}_s \\
\mathbf{k}_t \ &= \ \mathbf{k}_{p,out} + \|\mathbf{k}_{n,t}\| \mathbf{n}_s
\end{aligned}$$

A given order will only exist if the magnitude of the parallel (in-plane) wave vector is less than the magnitude of each out-going wave vector. That is

$$\|\mathbf{k}_{p,out}\| < k_0 n_1$$

for rays on the incoming side (reflected rays) and

$$\|\mathbf{k}_{p,out}\| < k_0 n_2$$

for rays on the outgoing side (transmitted rays). Each is equivalent to requiring one of the square roots in Equation 3-26 to return a positive real value.

### RELATIVE ORDER NUMBERS

For the **Grating** (but not the **Cross Grating**) it is possible to specify relative diffraction order numbers instead of absolute orders. This is particularly useful for blazed gratings.

In a blazed grating, the main detail of the grating microstructure is an array of facets that make an angle $\theta_B$ (SI unit: rad) with respect to the grating normal. This angle is known as the blaze angle. The absolute order number $m$ in which maximum diffraction efficiency occurs can be found from the general grating equation

$$m\lambda_0 = nd_g\cos\gamma(\sin\alpha + \sin\beta) ,$$

where the angles $\alpha$ and $\beta$ (SI unit: rad) are defined as

$$\alpha = \theta_B + \theta \qquad \beta = \theta_B - \theta'$$

where $\theta$ and $\gamma$ are the angles of incidence with respect to the grating normal in-plane and out-of-plane respectively. At the peak of the blaze function the angle of diffraction with respect to the grating normal ($\theta'$) is equal to $\theta$. Therefore, for any given wavelength $\lambda$, the absolute order number is given by

$$m = \text{round}\left[\frac{2nd_g}{\lambda}\cos\gamma\sin\theta_B\cos\theta\right] + \Delta m ,$$

where $\Delta m$ is the order number relative to the order in which this wavelength is closest to the blaze peak. The in-plane and out-of-plane angles can be derived from the incoming wave vector components. First, we have the component in the direction of the grating normal

$$k_n = \mathbf{k}\cdot\mathbf{n}_s .$$

The in-plane and out-of-plane components are

$$k_{p,\,in} = \mathbf{k}_p\cdot\mathbf{T}_g$$

and

$$k_{p,\,out} = \mathbf{k}_p\cdot(\mathbf{n}_s\times\mathbf{T}_g)$$

where $\mathbf{k}_p$ is the incoming wave vector projected onto the grating surface. This gives the angle $\theta$ and $\gamma$ as

$$\theta = -\text{atan}\left(\frac{k_{p,\,in}}{k_n}\right) - \theta_B$$

and

$$\gamma = -\text{atan}\left(\frac{k_{\text{p, out}}\cos\theta_B}{k_n}\right) .$$

## Ideal Lens Theory

The Ideal Lens feature can be used to treat a flat surface (in 3D) or an edge (in 2D) as if it were a lens, allowing it to focus or defocus rays.

*Optical Power*

The optical power $K$ (SI unit: $1/m$) of a lens is

$$K = \frac{1}{f_{\text{eff}}}$$

where $f_{\text{eff}}$ is the effective focal length (SI unit: m). For a thin lens, we have

$$K = K_1 + K_2$$

where

$$K_1 = \frac{n - n_1}{R_1} \quad K_2 = \frac{n - n_2}{R_2}$$

with $n_1$ and $n_2$ being the refractive index before and after the lens respectively, and where $n$ is the refractive index of the lens. The radii of curvature of the first and second lens surfaces is $R_1$ and $R_2$ (SI unit: m) respectively.

For a lens with thickness $T_c$ (SI unit: m), the optical power is instead

$$K = K_1 + K_2 + K_{12}$$

where

$$K_1 = \frac{n - n_1}{R_1} \quad K_2 = \frac{n - n_2}{R_2} \quad K_{12} = \frac{T_c}{n}K_1K_2$$

*Refracted Ray Direction*

For each point $\mathbf{r}$ (SI unit: m) on the lens surface, define an orthonormal coordinate system with unit vectors $\mathbf{e_r}$, $\mathbf{e_t}$, and $\mathbf{n_s}$ (the surface normal), where

$$\mathbf{e}_r = \frac{\delta \mathbf{r}}{|\delta \mathbf{r}|} \qquad \mathbf{e}_t = \mathbf{e}_r \times \mathbf{n}_s$$

where the subscripts $r$ and $t$ refer to the radial and tangential directions respectively. The distance $\delta \mathbf{r}$ is defined with respect to a reference point on the lens surface as $\delta \mathbf{r} = \mathbf{r} - \mathbf{r}_{ref}$.

The incoming ray direction can be split into the radial and tangential components as follows:

$$\tan \theta_{i, r} = \frac{\mathbf{n}_i \cdot \mathbf{e}_r}{\mathbf{n}_i \cdot \mathbf{n}_s} \qquad \tan \theta_{i, \phi} = \frac{\mathbf{n}_i \cdot \mathbf{e}_\phi}{\mathbf{n}_i \cdot \mathbf{n}_s} \ ,$$

where $\mathbf{n}_i$ is the incident ray direction. The ideal lens will only affect the radial component of the ray directions; that is

$$n_2 \tan \theta_r = n_1 \tan \theta_{i, r} - K|\delta \mathbf{r}|$$

and

$$n_2 \tan \theta_t = n_1 \tan \theta_{i, t}$$

and therefore the transmitted ray direction is

$$\mathbf{n}_t = \mathbf{n}_s + \tan \theta_r \mathbf{e}_r + \tan \theta_t \mathbf{e}_t$$

## Surface Scattering Theory

Several boundary features can be used to scatter rays. These include diffuse and isotropic reflection from a Wall, and perturbations due to surface slope error with an Illuminated Surface. These scattering models can be used in both transmission and/or reflection with the Scattering Boundary feature.

### DIFFUSE AND ISOTROPIC SCATTERING

Diffuse (or Lambertian) scattering follows the cosine law. That is, the flux $dn$ of rays across a surface element $A$ whose directions lie within a small solid angle $d\omega$ is proportional to the cosine of the polar angle $\theta$:

$$dn \propto A \cos \theta \, d\omega$$

or, substituting the expression for the differential solid angle,

$$d\omega = \sin \theta \, d\theta \, d\varphi$$

gives

$$dn \propto A \cos\theta \sin\theta \, d\theta \, d\varphi$$

where $\varphi$ is the azimuthal angle.

For isotropic scattering the flux of scattered rays is the same for any differential solid angle; that is

$$dn \propto A \, d\omega$$

or

$$dn \propto A \sin\theta \, d\theta \, d\varphi$$

*Diffuse and Isotropic Probability Distributions*

In 3D, the normalized probability distribution functions $f(\theta,\varphi)$ for diffuse and isotropic scattering are given by

$$f_{\text{diffuse}}(\theta, \varphi) = \frac{1}{\pi} \cos\theta \sin\theta \qquad f_{\text{isotropic}}(\theta, \varphi) = \frac{1}{2\pi} \sin\theta$$

where

$$\theta \in \left[0, \frac{\pi}{2}\right] \qquad \varphi \in [0, 2\pi]$$

In 2D these distributions become

$$f_{\text{diffuse}}(\theta) = \frac{1}{2} \cos\theta \qquad f_{\text{isotropic}}(\theta) = \frac{1}{\pi}$$

where

$$\theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right]$$

The direction components of a ray after it scatters diffusely or isotropically are given by

$$\begin{aligned}
\delta t_1 &= \sin\theta \cos\varphi \\
\delta t_2 &= \sin\theta \sin\varphi \\
\delta n &= \cos\theta
\end{aligned}$$

where $\delta n$ is the component in the direction of the surface normal ($\mathbf{n}_s$) and where $\delta t_1$ and $\delta t_2$ are the components in the two directions $\mathbf{t}_1$ and $\mathbf{t}_2$ orthogonal to the surface normal. That is, after scattering the reflected and transmitted ray directions are

$$\mathbf{n}_t = \delta t_1 \mathbf{t}_1 + \delta t_2 \mathbf{t}_2 + \delta n \mathbf{n}_s \qquad \mathbf{n}_r = \delta t_1 \mathbf{t}_1 + \delta t_2 \mathbf{t}_2 - \delta n \mathbf{n}_s$$

where

$$\mathbf{n}_s = \mathbf{t}_1 \times \mathbf{t}_2$$

### SURFACE SLOPE ERROR

Following Ref. 20 rays will be deviated upon reflection or refraction from a surface with a non-zero slope error. It will be assumed that the tangential deviation is negligible and that the radial distribution is Gaussian. Therefore, given an angular slope error $\sigma$, the probability distribution function for the polar angle is a Rayleigh distribution of the form

$$f(\theta) = \frac{\theta}{\sigma^2} \exp\left(-\frac{\theta^2}{2\sigma^2}\right) ,$$

which can be used to get the directions components $\delta n$, $\delta t_1$ and $\delta t_2$ as shown in the previous section. The effect of applying a surface slope error is to perturb the surface normal $\mathbf{n}_s$ to a value given by

$$\mathbf{n}_{s, p} = \delta t_1 \mathbf{t}_1 + \delta t_2 \mathbf{t}_2 + \delta n \mathbf{n}_s$$

form which the equations of reflection and refraction proceed as normal.

## *Volumetric Scattering Theory*

The Scattering Domain feature is used to model the interaction of rays with a dilute phase of particles in the medium the rays pass through. Some examples of this include the following:

- Water droplets, smoke, or dust in air,
- Bubbles in water, and
- Colloidal suspensions of metallic nanoparticles in water.

### TYPES OF SCATTERING BEHAVIOR

When a beam of light passes through a cloud of particles, some energy is subtracted from the forward-propagating beam. Two other things can happen to the subtracted

energy: it is either sent out in a different direction (scattering) or converted into another form of energy within the particles, most often heat (absorption). The overall subtraction of energy from the forward-propagating direction is called extinction. By the principle of conservation of energy, the fundamental relationship between the different scattering phenomena is

$$\text{extinction} = \text{scattering} + \text{absorption} \tag{3-27}$$

**PROPERTIES OF SCATTERING PARTICLES**

The scattering particles are assumed to be homogeneous isotropic spheres. The space between them is assumed to be large compared to the electromagnetic wavelength and particle size. In addition, the particles are also assumed to be oriented randomly, not in any specific pattern (such as a rectangular array). Thus there is no coherent phase relationship between different particles, so scattering by many particles can be understood by first considering a single isolated sphere.

Simplifying assumptions can be made if the particles are very large or very small when compared to the wavelength of the electromagnetic radiation. When the particles are optically very small, the simplified Rayleigh scattering model can be used. For particles much larger than the wavelength, the ratio of extinction cross section to geometrical cross section approaches an asymptotic limit of 2.

When the particles are neither optically very large nor very small, the more general Mie scattering theory must be used. Mie theory provides an exact solution for the interaction of a plane wave with a sphere, but the calculations involved are much more computationally intensive than either of the asymptotic limits for large or small particles.

When considering whether the particles are small enough to apply Rayleigh theory, remember to consider the wavelength both inside and outside the particle; this could make a big difference if the particles are made of a highly conductive material.

**CROSS SECTIONS AND EFFICIENCY FACTORS**

Let $n_p$ (dimensionless) be the absolute refractive index of a spherical particle, and $n_a$ (dimensionless) the absolute refractive index of the surrounding medium. For this analysis, $n_a$ is assumed to be real (non-absorbing) but $n_p$ may be complex-valued,

$$n_p = n_{p,r} - i n_{p,i}$$

where $n_{p,i} > 0$ for absorbing particles.

The wavelength in the medium surrounding the particle $\lambda$ (SI unit: m) is

$$\lambda = \frac{\lambda_0}{n_a}$$

where $\lambda_0$ (SI unit: m) is the vacuum wavelength.

For optical scattering calculations, it is convenient to work with dimensionless variables, such as the dimensionless size parameter $x$,

$$x = \frac{2\pi R}{\lambda}$$

where $R$ (SI unit: m) is the radius of the scattering particle.

The size parameter may also be expressed in terms of the wave number in the surrounding medium $k$ (SI unit: rad/m),

$$k = \frac{2\pi}{\lambda}$$

Thus,

$$x = kR$$

For brevity, in the remainder of this section the relative refractive index of the scattering particle, that is, the ratio of the particle refractive index to that of the surroundings, will be denoted $n$,

$$n \equiv \frac{n_p}{n_a}$$

although caution should be used because $n$ denotes the absolute index in other sections of this manual.

Consider an incident beam of light with cross sectional area $A_0$ (SI unit: m$^2$) and intensity $I_0$ (SI unit: W/m$^2$). This beam illuminates a surface, conferring an amount of energy equal to $I_0 A_0$. Now suppose that a single spherical particle obstructs part of the beam, so that the energy reaching the surface is now $I_0 A_1$. Then the difference $A_0$ - $A_1$ is the extinction cross section $\sigma_{ext}$ (SI unit: m$^2$) of the particle.

In other words, the extinction cross section of a particle is the surface area on a detector that, if subtracted, causes the same reduction in total energy at that detector as the presence of the particle in the beam.

Looking closer at the particle, the extinction or energy removal can be separated into two phenomena: scattering and absorption. The amount of energy absorbed by the

particle and converted to other forms of energy (predominantly heat) is $I_0\sigma_{abs}$, where $I_0\sigma_{abs}$ (SI unit: $m^2$) is the absorption cross section. The amount of energy that radiates outward from the particle in directions other than the direction of the incident beam is $I_0\sigma_{sca}$, where $\sigma_{sca}$ (SI unit: $m^2$) is the scattering cross section.

By the principle of conservation of energy exemplified in Equation 3-27, the three cross sections follow the relationship

$$\sigma_{ext} = \sigma_{sca} + \sigma_{abs} \tag{3-28}$$

For each cross section, it is convenient to define a dimensionless efficiency factor by dividing by the geometrical cross-sectional area of the particle,

$$Q_{ext} = \frac{\sigma_{ext}}{\pi R^2} \qquad Q_{sca} = \frac{\sigma_{sca}}{\pi R^2} \qquad Q_{abs} = \frac{\sigma_{abs}}{\pi R^2} \tag{3-29}$$

where

- $Q_{ext}$ is the extinction efficiency,
- $Q_{sca}$ is the scattering efficiency, and
- $Q_{abs}$ is the absorption efficiency.

Like the scattering cross sections, the efficiency factors follow a relationship based on the energy conservation principle,

$$Q_{ext} = Q_{sca} + Q_{abs} \tag{3-30}$$

It is convenient describe the scattering behavior in terms of the dimensionless quantities $x$, $Q_{ext}$, $Q_{sca}$, and $Q_{abs}$, rather than the particle radius, wavelength, and cross sections. Another dimensionless variable is sometimes needed: the product of the size parameter with the relative refractive index is denoted $y$,

$$y \equiv nx$$

### RAYLEIGH SCATTERING THEORY

Rayleigh scattering theory (not to be confused with Rayleigh-Gans theory) is a simplified scattering model for optically small particles. For Rayleigh scattering theory to be applicable, the particle must be small relative to the wavelength outside of it,

$$x \ll 1$$

and also small relative to the wavelength inside it,

$$|n|x \ll 1$$

It is possible for the former to be true, but not the latter, if the scattering centers are small metallic particles with refractive indices that have very large imaginary parts.

The scattering and absorption efficiency factors in the Rayleigh limit are

$$Q_{\text{sca}} = \frac{8}{3}x^4\left|\frac{n^2-1}{n^2+2}\right|^2 \tag{3-31}$$

$$Q_{\text{abs}} = -4x\,\text{Im}\left(\frac{n^2-1}{n^2+2}\right) \tag{3-32}$$

As usual, the sum of these two efficiency factors yields the extinction efficiency factor.

The absorption efficiency factor is thus zero if the refractive index of the scattering particles is real-valued. However, if the refractive index has any imaginary part, the absorption efficiency factor tends to dominate because it is only proportional to the first power of the size parameter $x$, whereas the scattering efficiency scales with the fourth power of $x$; when applying Rayleigh scattering theory, $x$ tends to be very small.

### MIE SCATTERING THEORY

The Mie scattering theory represents an exact solution to the scattering of a plane wave by a homogeneous, isotropic spherical particle. In principle, this exact solution can be used for any value of the size parameter $x$. In practice, some expressions for the efficiency factors can become ill-conditioned or numerically unstable at extremely large or small $x$, or if the refractive index has a very large imaginary part.

A complete derivation for the scattering amplitudes will not be given here; instead, the reader is directed to Ref. 20. The extinction and scattering efficiency factors are defined as infinite series,

$$Q_{\text{ext}} = \frac{2}{x^2}\sum_{l=1}^{\infty}(2l+1)\text{Re}(a_l+b_l) \tag{3-33}$$

$$Q_{\text{sca}} = \frac{2}{x^2}\sum_{l=1}^{\infty}(2l+1)(|a_l|^2+|b_l|^2) \tag{3-34}$$

The absorption efficiency factor if the difference between these two expressions. The coefficients $a_l$ and $b_l$ are expressions involving the Riccatti–Bessel functions

$$a_l = \frac{\psi_l'(y)\psi_l(x) - n\psi_l(y)\psi_l'(x)}{\psi_l'(y)\zeta_l(x) - n\psi_l(y)\zeta_l'(x)}$$

$$b_l = \frac{n\psi_l'(y)\psi_l(x) - \psi_l(y)\psi_l'(x)}{n\psi_l'(y)\zeta_l(x) - \psi_l(y)\zeta_l'(x)}$$

(3-35)

These functions can be expressed in terms of the spherical Bessel functions of the first and third kind, or in terms of the corresponding Bessel functions,

$$\psi_l(x) = xj_l(x) = \sqrt{\frac{\pi x}{2}}J_{l+1/2}(x)$$

$$\zeta_l(x) = xh_l^{(2)}(x) = \sqrt{\frac{\pi x}{2}}H_{l+1/2}^{(2)}(x)$$

---

📝 In Ref. 21, spherical Hankel functions of the first kind $h_l^{(1)}(x)$ are used. This is tied to the author's choice of sign convention when setting up the electromagnetic wave equation. The convention used in COMSOL is generally to represent the transient part of an electromagnetic wave as $\exp(i\omega t)$, whereas Ref. 21 uses $\exp(-i\omega t)$. Ref. 20 uses $\exp(i\omega t)$ and also arrives at $h_l^{(2)}(x)$.

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The primes in Equation 3-35 indicate differentiation with respect to the argument of the function,

$$\psi_l'(y) = \frac{d\psi_l(y)}{dy} \qquad \psi_l'(y) = \frac{d\psi_l(y)}{dy}$$

$$\zeta_l'(x) = \frac{d\psi_l(x)}{dx} \qquad \zeta_l'(y) = \frac{d\psi_l(y)}{dy}$$

The general workflow of Mie scattering calculation is to first compute the Riccatti-Bessel functions $\psi_l$ and $\zeta_l$; then the scattering coefficients $a_l$ and $b_l$; and finally the scattering efficiency factors $Q_{ext}$ and $Q_{sca}$.

---

💡 The scattering efficiency factors are computed using the built-in COMSOL functions `mieextinction(n,x)` and `miescattering(n,x)`. The first input argument is the relative refractive index of the scattering particle and the second input argument is the size parameter. Although primarily used in ray optics, these functions can be accessed in any model.

---

Efficient evaluation of the efficiency factors from Mie theory means that the scattering coefficients $a_l$ and $b_l$ from Equation 3-35 must be computed as quickly and robustly as possible. Although they are infinite series, in practice the terms start to become negligibly small when the index $l$ is somewhat larger than $x$, so the series can be taken to a finite upper bound $L$; one recommendation for the value of L (Ref. 21) is

$$L = x + 4x^{1/3} + 2$$

For example, if the size parameter is 1000, the first 1042 terms in the infinite series will be computed.

*Recurrence Relations*

One approach to computing the scattering coefficients is via upward recurrence. The first few Riccatti-Bessel functions are

$$\psi_{-1}(x) = \cos x \qquad\qquad \psi_0(x) = \sin x$$
$$\zeta_{-1}(x) = \cos x - i\sin x \qquad \zeta_0(x) = \sin x + i\cos x$$

and the remainder can be obtained via the recurrence relations

$$\psi_{l+1}(x) = \frac{2l+1}{x}\psi_l(x) - \psi_{l-1}(x)$$
$$\zeta_{l+1}(x) = \frac{2l+1}{x}\zeta_l(x) - \zeta_{l-1}(x)$$

## LARGE CONDUCTING SPHERES: THE EXTINCTION PARADOX

When scattering particles are very large ($x \gg 1000$), the extinction efficiency factor from Mie theory asymptotically approaches a value of 2. In other words, the extinction cross section of a large particle is double its geometrical cross section.

This observation is sometimes called the extinction paradox because it is contrary to most day-to-day observations, in which a large object only obstructs the light that intersects its geometrical cross section.

The apparent contradiction can be resolved (see for example Ref. 20) by noting that the interpretation of the extinction cross section requires observation of the scattered light to be made at a very large distance from the scattering particle, where regions of light and shadow are not so distinct. According to Babinet's principle, when a certain amount of light is blocked by the surface of an object, an equal amount of light is diffracted around the edges of the object. For close-range interactions such as light illuminating a piece of furniture in a room, it is extremely difficult to distinguish the diffracted light from the light that continues in the forward scattering direction ($\theta = 0$)

because the diffracted light concentrated in a very narrow cone about the forward scattering direction. The scattering amplitudes for diffracted light as a function of scattering angle are

$$S_1^{(d)}(\theta) = S_2^{(d)}(\theta) = x^2 \frac{J_1(x \sin \theta)}{x \sin \theta}$$

where $J_1$ is the Bessel function of the first kind; so if $x$ is very large, most of the energy is contained within a very small angle.

## Interference Pattern Theory

The **Interference Pattern** plot can be used to visualize the fringes resulting from the interference of two or more rays at a surface. The interference pattern is only valid when it is plotted over an area with a length scale that is much smaller than the principal radius of curvature of any incident wavefront. This is a consequence of the treatment of each ray as a wavefront that subtends a small solid angle. Furthermore, this plot type requires calculation of the ray intensity and instantaneous phase.

Given the phase $\Psi_0$ of a ray at the point $(q_x, q_y)$ where the ray intersects a plane, the phase $\Psi$ at a nearby point $(q_x + \Delta x, q_y + \Delta y)$ is computed as follows. Without loss of generality assume that the $x$- and $y$-axes are oriented so that they are parallel to the projections of the principal curvature directions onto the cut plane. For a spherical wavefront, the orientations of these axes may be determined arbitrarily as long as they are orthogonal. Let $n_{i,x}$ and $n_{i,y}$ denote the $x$- and $y$- components, respectively, of the normalized ray direction vector. Let $r_1$ and $r_2$ denote the principal radii of curvature in the directions parallel to the $x$- and $y$-axes, respectively. For an incident ray with wave vector magnitude $k$, the phase at $(q_x + \Delta x, q_y)$ is

$$\Psi(q_x + \Delta x, q_y) = \Psi(q_x, q_y) + k \Delta r_1$$

Where $\Delta r_1$ is the change in the principal radius of curvature of the wavefront when moving between the two points.

$$(r_1 + \Delta r_1)^2 = [r_1^2 - (n_{i,x} r_1)^2] + (n_{i,x} r_1 + \Delta x)^2$$

Further simplification yields

$$\Delta r_1 = \sqrt{r_1^2 + 2 n_{i,x} r_1 \Delta x + \Delta x^2} - r_1$$

This equation yields an indeterminate form in the limit of infinite radii of curvature, making it unsuitable for computing interference patterns involving plane waves. The equation can be made more robust for plane waves by applying a Taylor series approximation about $\Delta x = 0$,

$$\sqrt{r_1^2 + 2n_{i,x}r_1\Delta x + \Delta x^2} = r_1 + n_{i,x}\Delta x + \frac{1}{2r_1}(1 - n_{i,x}^2)\Delta x^2 + O(\Delta x^3)$$

Discarding terms of order $\Delta x^3$ or higher yields

$$\Delta r_1 = n_{i,x}\Delta x + \frac{1}{2r_1}(1 - n_{i,x}^2)\Delta x^2$$

Similarly, the change in principal radius of curvature due to a small perturbation in the $y$ direction is

$$\Delta r_2 = n_{i,y}\Delta y + \frac{1}{2r_2}(1 - n_{i,y}^2)\Delta y^2$$

The rationale for discarding higher-order terms is that they all involve division by higher powers of $r_1$ and $r_2$. Therefore this series approximation is only valid when the perturbations in the $x$ and $y$ directions are much smaller than the principal radii of curvature. To assume otherwise would mean that the incident wavefronts subtend very large solid angles.

Combining the perturbations in the two principal radii of curvature yields an expression for the phase at any point $(q_x + \Delta x, q_y + \Delta y)$ on the cut plane,

$$\Psi = \Psi_0 + k\left[n_{i,x}\Delta x + \frac{1}{2r_1}(1 - n_{i,x}^2)\Delta x^2 + n_{i,y}\Delta y + \frac{1}{2r_2}(1 - n_{i,y}^2)\Delta y^2\right]$$

The incident Stokes vector is then converted to an incident electric field using the relation

$$I = \frac{n}{2}\sqrt{\frac{\varepsilon_0}{\mu_0}}(\mathbf{E} \cdot \mathbf{E}^*)$$

and the electric field at the intersection of the ray with the cut plane can be used to compute the electric field at a nearby point using the relation

$$\mathbf{E}(q_x + \Delta x, q_y + \Delta y) = \mathbf{E}(q_x, q_y)\exp[\Psi(q_x + \Delta x, q_y + \Delta y) - \Psi_0]$$

where it is again assumed that the ray subtends a small solid angle so that the intensity of the incident ray is approximately uniform over the region in which the interference pattern is plotted. It is then straightforward to compute the sum of the electric fields of all incident rays and derive the total incident intensity from the electric field norm.

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🔍     Results Analysis and Visualization in the Ray Optics Modeling chapter.

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### Monochromatic Aberrations and the Zernike Polynomials

A standard way to quantify monochromatic aberrations is to express the optical path difference of all incident rays as a linear combination of Zernike polynomials. With the Ray Optics Module, the Zernike coefficients can be reported in a table using the **Aberration Evaluation** feature. Alternatively, a superposition of different Zernike polynomials can be shown on a unit circle using the **Optical Aberration** plot.

Several different standards exist for naming, normalizing, and organizing the Zernike polynomials. The approach used in this section follows the standards published by the International Organization for Standardization (ISO, Ref. 23) and the American National Standards Institute (ANSI, Ref. 24).

Each Zernike polynomial $Z_n^m$ can be expressed as

$$Z_n^m = N_n^m R_n^{|m|}(\rho) M(m\theta)$$

where

- $N_n^m$ is the normalization term,
- $R_n^{|m|}$ is the radial term,
- $M(m\theta)$ is the meridional term or azimuthal term,
- $\rho$ is the radial parameter, given by $\rho = r/a$ where $r$ is the distance from the aperture center and $a$ is the aperture radius, so that $0 \leq \rho \leq 1$,
- $\theta$ is the meridional parameter or azimuthal angle, $0 \leq \theta \leq 2\pi$,
- the lower index $n$ is a nonnegative integer, $n = 0,1,2,\ldots$, and
- the upper index $m$ is an integer, $m = -n, -n + 2, \ldots, n - 2, n$ so that $n - |m|$ is always even.

The normalization term $N_n^m$ is

$$N_n^m = (2 - \delta_{0,m})(n + 1)$$

where $\delta_{0,m}$ is the Kronecker delta,

$$\delta_{i,j} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

The radial term is given by the equation

$$R_n^m(\rho) = \sum_{s=0}^{0.5(n - |m|)} \frac{(-1)^s (n - s)!}{s![0.5(n + |m|) - s]![0.5(n - |m|) - s]!} \rho^{n - 2s}$$

where "!" denotes the factorial operator; for nonnegative integers,

$$n! = \begin{cases} 1 & n = 0 \\ 1 \times 2 \times 3 \times \ldots \times n & n > 0 \end{cases}$$

The meridional term is given by the equation

$$M(m\theta) = \begin{cases} \cos(m\theta) & m \geq 0 \\ \sin(|m|\theta) & m < 0 \end{cases}$$

The Zernike polynomials thus defined are normalized Zernike polynomials. They are orthogonal in the sense that any pair of Zernike polynomials satisfy the equation

$$\int_0^1 \rho d\rho \int_0^{2\pi} Z_n^m Z_{n'}^{m'} d\theta = \pi \delta_{n,n'} \delta_{m,m'}$$

The normalized Zernike polynomials up to fifth order, along with their common names, are given in Table 3-4.

TABLE 3-4:  ZERNIKE POLYNOMIALS

| TERM | EXPRESSION | COMMON NAME |
|------|------------|-------------|
| $Z_0^0$ | 1 | Piston |
| $Z_1^{-1}$ | $2\rho \sin(\theta)$ | Vertical tilt |
| $Z_1^1$ | $2\rho \cos(\theta)$ | Horizontal tilt |

TABLE 3-4: ZERNIKE POLYNOMIALS

| TERM | EXPRESSION | COMMON NAME |
|---|---|---|
| $Z_2^{-2}$ | $\sqrt{6}\rho^2\sin(2\theta)$ | Oblique astigmatism |
| $Z_2^0$ | $\sqrt{3}(2\rho^2-1)$ | Defocus |
| $Z_2^2$ | $\sqrt{6}\rho^2\cos(2\theta)$ | Astigmatism |
| $Z_3^{-3}$ | $\sqrt{8}\rho^3\sin(3\theta)$ | Oblique trefoil |
| $Z_3^{-1}$ | $\sqrt{8}(3\rho^3-2\rho)\sin(\theta)$ | Vertical coma |
| $Z_3^1$ | $\sqrt{8}(3\rho^3-2\rho)\cos(\theta)$ | Horizontal coma |
| $Z_3^3$ | $\sqrt{8}\rho^3\cos(3\theta)$ | Horizontal trefoil |
| $Z_4^{-4}$ | $\sqrt{10}\rho^4\sin(4\theta)$ | Oblique quatrefoil |
| $Z_4^{-2}$ | $\sqrt{10}(4\rho^4-3\rho^2)\sin(2\theta)$ | Oblique secondary astigmatism |
| $Z_4^0$ | $\sqrt{5}(6\rho^4-6\rho^2+1)$ | Spherical aberration |
| $Z_4^2$ | $\sqrt{10}(4\rho^4-3\rho^2)\cos(2\theta)$ | Secondary astigmatism |
| $Z_4^4$ | $\sqrt{10}\rho^4\cos(4\theta)$ | Horizontal quatrefoil |
| $Z_5^{-5}$ | $\sqrt{12}\rho^5\sin(5\theta)$ | |
| $Z_5^{-3}$ | $\sqrt{12}(5\rho^5-4\rho^3)\sin(3\theta)$ | |
| $Z_5^{-1}$ | $\sqrt{12}(10\rho^5-12\rho^3+3\rho)\sin(\theta)$ | |
| $Z_5^1$ | $\sqrt{12}(10\rho^5-12\rho^3+3\rho)\cos(\theta)$ | |
| $Z_5^3$ | $\sqrt{12}(5\rho^5-4\rho^3)\cos(3\theta)$ | |
| $Z_5^5$ | $\sqrt{12}\rho^5\cos(5\theta)$ | |
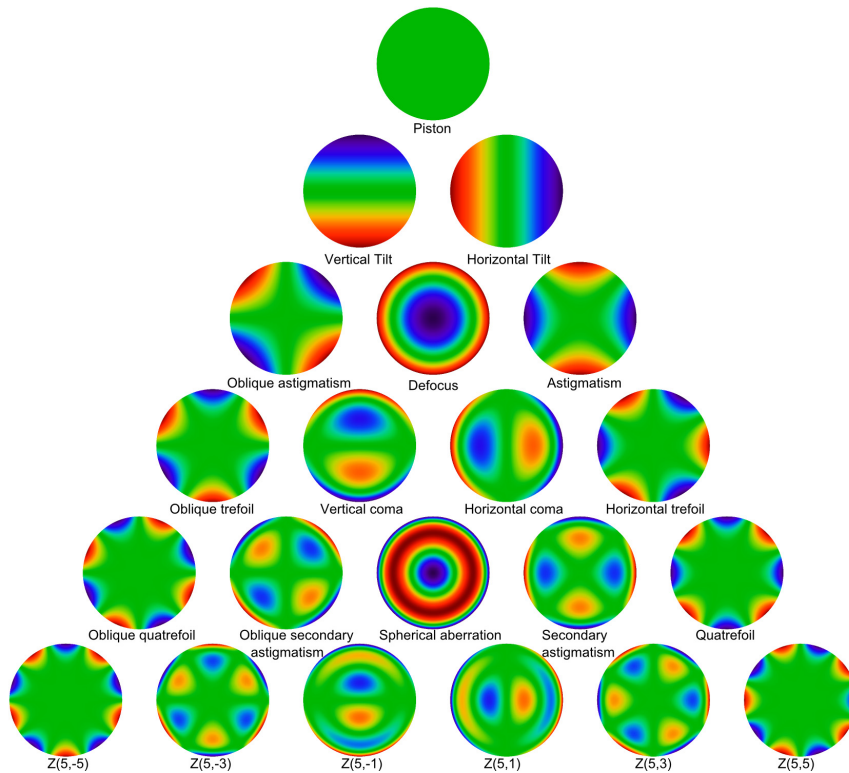
*Figure 3-14: Zernike polynomials on the unit circle.*

## Accumulator Theory: Domains

The Accumulator (Domain) node is used to transfer information from rays to the domains they occupy or pass through. Each **Accumulator** defines a variable, called the accumulated variable, in the selected domains. The accumulated variable is discretized using constant shape functions, so its value is uniform over every mesh element and may be discontinuous between adjacent mesh elements.

The name of the accumulated variable is specified in the **Accumulated variable name** field in the **Accumulator Settings** section of the settings window. The default variable name, **rpd**, will be used in the remainder of this section when referring to the accumulated variable.

## ACCUMULATOR TYPE

The options in the **Accumulator type** list are **Density** and **Count**. If **Density** is selected, the source term is divided by the area or volume of the mesh element when calculating each ray's contribution to the accumulated variable. If **Count** is selected, no division by the area or volume of the mesh element occurs.

The equations in the following section are valid for the **Density** type. The corresponding value of the accumulated variable for the **Count** type is

$$\mathrm{rpd}_{\mathrm{count}} = \mathrm{rpd}_{\mathrm{density}} \times V$$

where $V$ is the mesh element volume (in 3D) or area (in 2D).

## ACCUMULATION OVER ELEMENTS

When **Elements** is selected from the **Accumulate over** list, the value of the accumulated variable in a mesh element is the sum of the source terms $R_i$ evaluated for all rays in that mesh element:

$$\mathrm{rpd} = \frac{1}{V} \sum_{i=1}^{N} R_i$$

where $N$ is the total number of rays in the element and $V$ is the area or volume of the mesh element. In other words, the contribution of each ray to the accumulated variable is distributed uniformly over the mesh element the ray is in, regardless of the ray's exact position within the element.

If **Elements and time** is selected from the **Accumulate over** list, then the sum of the source terms for rays in the mesh element is used to define the time derivative of the accumulated variable, rather than its instantaneous value:

$$\frac{d(\mathrm{rpd})}{dt} = \frac{1}{V} \sum_{i=1}^{N} R_i$$

Thus the value of the accumulated variable depends on the time history of rays in the mesh element, instead of the instantaneous positions of the rays. As each ray propagates, it will leave behind a trail based on its contributions to the accumulated variables in mesh elements it has traversed. The algorithm for accumulating over time takes into account the fraction of a time step taken by the solver that the ray spends in each mesh element, even if it crosses between elements during the time step.

## Accumulator Theory: Boundaries

The Accumulator (Boundary) feature transfers information from rays to the boundaries they hit or pass through. Each **Accumulator** defines a variable, called the accumulated variable, on the selected boundaries. The accumulated variable is discretized using constant shape functions, so its value if uniform over every mesh element and may be discontinuous between adjacent mesh elements.

The name of the accumulated variable is specified in the **Accumulated variable name** field in the **Accumulator Settings** section of the settings window. The default variable name, rpb, will be used in the remainder of this section when referring to the accumulated variable.

The options in the **Accumulator type** list are **Density** and **Count**. If **Density** is selected, the source term is divided by the surface area or length of the boundary mesh element when calculating each ray's contribution to the accumulated variable. If **Count** is selected, no division by the surface area or length of the boundary element occurs.

The equations in the following section are valid for the **Density** type. The corresponding value of the accumulated variable for the **Count** type is

$$rpb_{count} \ = \ rpb_{density} \times V$$

where $V$ is the boundary element surface area (in 3D) or length (in 2D).

When **Rays in boundary elements** is selected from the **Accumulate over** list, the accumulated variable in a boundary element gets incremented by the source term $R$ whenever a ray freezes or sticks to the boundary:

$$rpb_{new} \ = \ rpb + \frac{R}{V}$$

where division by the mesh element area or length occurs because the accumulator is assumed to be of type **Density**. Thus the source term evaluated for an incident ray is uniformly distributed over the boundary element it freezes or sticks to.

If instead **Ray-wall interactions** is selected from the **Accumulate over** list, then the accumulated variable gets incremented regardless of what type of ray-wall interaction occurs. Thus, it is possible for the same ray to increment the accumulated variable in many different boundary elements, or even in the same element multiple times.

**BUILT-IN GLOBAL VARIABLES**

By default, the boundary **Accumulator** defines the following global variables:

TABLE 3-5:  BUILT-IN GLOBAL VARIABLES FOR BOUNDARY ACCUMULATORS

| NAME | EXPRESSION |
|---|---|
| `<scope>.<name>_ave` | Average of accumulated variable |
| `<scope>.<name>_int` | Integral of accumulated variable |
| `<scope>.<name>_max` | Maximum of accumulated variable |
| `<scope>.<name>_min` | Minimum of accumulated variable |
| `<scope>.<name>_sum` | Sum of accumulated variable over elements |

Here, `<scope>` includes the physics interface name and the names the Accumulator and parent feature. For example, the average of the accumulated variable over a boundary may be called `gop.wall1.bacc1.rpb_ave`, where `gop` is the name of the Geometrical Optics interface, `wall1` is the name of the parent Wall node, `bacc1` is the name of the Accumulator node, and `rpb` is the accumulated variable name. These variables are all available in the **Add/Replace Expression** menus during results evaluation.

These global variables are computed by defining a set of nonlocal couplings on the selection of the parent physics feature, such as the Wall feature to which the Accumulators are added. The following expressions for the global variables are used.

TABLE 3-6:  BUILT-IN GLOBAL VARIABLE DEFINITIONS FOR BOUNDARY ACCUMULATORS

| NAME | EXPRESSION |
|---|---|
| `<scope>.<name>_ave` | `<wscope>.aveop(<scope>.<name>)` |
| `<scope>.<name>_int` | `<wscope>.intop(<scope>.<name>)` |
| `<scope>.<name>_max` | `<wscope>.maxop(<scope>.<name>)` |
| `<scope>.<name>_min` | `<wscope>.minop(<scope>.<name>)` |
| `<scope>.<name>_sum` | `<wscope>.intop(<scope>.<name>/<scope>.meshVol)` |

Here, `<wscope>` is the scope of the parent boundary feature, for example, `gop.wall1`.

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# 4

# Multiphysics Interfaces and Couplings

The Ray Optics Module contains predefined multiphysics interfaces and couplings to facilitate easy setup of models of ray propagation with significant attenuation and heating. The **Ray Heating** physics interface described in this chapter is found under the **Optics>Ray Optics** branch ( ) when adding a physics interface.

In this chapter:

- The Ray Heating Interface
- Theory for the Ray Heating Interface

# The Ray Heating Interface

The **Ray Heating** interface ( ) combines the Geometrical Optics interface with the Heat Transfer in Solids interface. The **Ray Heat Source** multiphysics feature is added automatically. The Ray Heating interface is used to model electromagnetic wave propagation in optically large systems in which the refractive index is temperature dependent. The energy lost due to the attenuation of rays in an absorbing medium creates a heat source that is included in the temperature computation.

When a predefined **Ray Heating** interface is added from the **Optics>Ray Optics** branch ( ) of the **Model Wizard** or **Add Physics** windows, **Geometrical Optics** and **Heat Transfer in Solids** interfaces are added to the Model Builder. A **Multiphysics** node is also added, which automatically includes the multiphysics coupling feature **Ray Heat Source**.

*On the Constituent Physics Interfaces*
The Geometrical Optics interface is used to model electromagnetic wave propagation when the wavelength is much smaller than the smallest geometric entity in the model. It includes built-in tools for computing the intensity, phase, and optical path length of rays. The rays can be polarized, unpolarized, or partially polarized. Frequency distributions and ray propagation in absorbing media are also supported.

The Heat Transfer in Solids interface is used to model heat transfer by conduction, convection, and radiation. A Heat Transfer in Solids model is active by default on all domains and a Heat Transfer in Fluids model is added with an empty selection. All functionality for including other domain types, such as a fluid domain, is also available. The temperature equation defined in solid domains corresponds to the differential form of the Fourier's law that may contain additional contributions like heat sources.

### SETTINGS FOR PHYSICS INTERFACES AND COUPLING FEATURES
When physics interfaces are added using the predefined couplings, for example **Ray Heating**, specific settings are included with the physics interfaces and the coupling features.

However, if physics interfaces are added one at a time, followed by the coupling features, these modified settings are not automatically included.

For example, if single **Geometrical Optics** and **Heat Transfer in Solids** interfaces are added, COMSOL adds an empty **Multiphysics** node. You can choose from the available coupling features but the modified settings are not included.

| | Coupling features are available from the context menu (right-click the **Multiphysics** node) or from the **Physics** toolbar, **Multiphysics** menu. |
|---|---|

TABLE 4-1: MODIFIED SETTINGS FOR A RAY HEATING INTERFACE

| PHYSICS INTERFACE OR COUPLING FEATURE | MODIFIED SETTINGS (IF ANY) |
|---|---|
| Geometrical Optics | **Compute intensity and power** is selected from the **Intensity computation** list in the physics interface **Ray Properties** section. |
| Heat Transfer in Solids | No changes. |
| Ray Heat Source | The **Domain Selection** is the same as that of the participating physics interfaces. <br><br> The corresponding Geometrical Optics and Heat Transfer in Solids interfaces are preselected in the **Ray Heat Source** section. |

### PHYSICS INTERFACES AND COUPLING FEATURES

| | Use the online help in COMSOL Multiphysics to locate and search all the documentation. All these links also work directly in COMSOL Multiphysics when using the Help system. |
|---|---|

*Coupling Features*
The Ray Heat Source coupling feature node is described in this section.

*Physics Interface Features*
Physics nodes are available from the **Physics** ribbon toolbar (Windows users), **Physics** context menu (Mac or Linux users), or right-click to access the context menu (all users).

| | In general, to add a node, go to the **Physics** toolbar, no matter what operating system you are using. Subnodes are available by clicking the parent node and selecting it from the **Attributes** menu. |
|---|---|

- The available physics features for The Geometrical Optics Interface are listed in the section List of Geometrical Optics Interface Physics Features.

- The available physics features for The Heat Transfer Interfaces are listed in the sections Domain Features, Boundary Features, and Edge and Point Features in the *COMSOL Multiphysics Reference Manual*.

## Ray Heat Source

Use the **Ray Heat Source** multiphysics coupling ( ) to compute the heat source resulting from the attenuation of rays in an absorbing medium. This heat source is defined to a dependent variable that is defined on all domain mesh elements in the selection of the **Ray Heat Source** node. The ray power should be solved for in the coupled Geometrical Optics interface.

### SETTINGS

The **Label** is the default multiphysics coupling name.

The **Name** is used primarily as a scope prefix for variables defined by the coupling node. Refer to such variables in expressions using the pattern <name>.<variable_name>. In order to distinguish between variables belonging to different coupling nodes or physics interfaces, the name string must be unique. Only letters, numbers, and underscores (_) are permitted in the **Name** field. The first character must be a letter.

The default **Name** (for the first multiphysics coupling in the model) is rhs1.

### RAY HEAT SOURCE

This section defines the physics involved in the multiphysics coupling. By default, the applicable physics interface is selected in the **Source** and **Destination** lists.

You can also select **None** from either list to uncouple the node from a physics interface. If the physics interface is removed from the **Model Builder** then the applicable list defaults to **None** as there is nothing to couple to.

| | If a physics interface is deleted and then added to the model again, and in order to reestablish the coupling, you need to choose the physics interface again from the **Source** or **Destination** lists. This is applicable to all multiphysics coupling nodes that would normally default to the once present physics interface. See Multiphysics Modeling Workflow in the *COMSOL Multiphysics Reference Manual*. |
|---|---|

# Theory for the Ray Heating Interface

The Ray Heating Interface theory is described in this section:

- Unidirectional and Bidirectional Couplings
- Coupled Heat Transfer and Ray Tracing Equations
- Heat Source Calculation

## *Unidirectional and Bidirectional Couplings*

The Ray Heating multiphysics interface combines geometrical optics with heat transfer to compute the heat source that is generated as rays propagate through an absorbing medium. The Ray Heating interface can either be used to set up a unidirectional or bidirectional coupling between the constituent physics interfaces.

If the medium properties are not temperature dependent and the domains do not undergo significant thermal expansion, then a unidirectional coupling is appropriate. The heat source generated by the attenuation of rays can be included in the heat transfer simulation by first computing the ray trajectories using a Ray Tracing study step, then computing the temperature using a Stationary study step. Both study steps are described in the *COMSOL Multiphysics Reference Manual.*

If the refractive index of the medium is temperature dependent, a more accurate approach is to set up a bidirectional coupling in which the attenuation of ray power affects the temperature distribution, which in turn affects the ray trajectories. The two physics can be solved for using an iterative solver loop consisting of a time-dependent solver for the ray trajectories and a stationary solver for the temperature. Such a solver sequence can be set up automatically using the Bidirectionally Coupled Ray Tracing study step, also described in the *COMSOL Multiphysics Reference Manual.*

## *Coupled Heat Transfer and Ray Tracing Equations*

Under static conditions, the heat equation can be written as

$$\rho C_p \mathbf{u} \cdot \nabla T + \nabla \cdot \mathbf{q} = Q$$

$$\mathbf{q} = -k\nabla T$$

where

- $\rho$ (SI unit: kg/m$^3$) is the density,
- $C_p$ (SI unit: J/(kg·K)) is the heat capacity at constant pressure,
- $T$ (SI unit: K) is the temperature,
- $Q$ (SI unit: W/m$^3$) is the heat source, and
- $k$ (SI unit: W/(m·K)) is the thermal conductivity.

The propagation of each ray can be modeled using a set of coupled first-order equations:

$$\frac{d\mathbf{k}}{dt} = -\frac{\partial\omega}{\partial\mathbf{q}} \qquad \frac{d\mathbf{q}}{dt} = \frac{\partial\omega}{\partial\mathbf{k}}$$

where $\mathbf{k}$ (SI unit: rad/m) is the wave vector, $\omega$ (SI unit: rad/s) is the angular frequency, $t$ (SI unit: s) is time, and $\mathbf{q}$ (SI unit: m) is the ray position vector. In an isotropic medium, the frequency and wave vector are related by the expression

$$\omega = \frac{c|\mathbf{k}|}{n(\mathbf{q})}$$

where $c$ = 299,792,458 m/s is the speed of light in a vacuum and $n$ (dimensionless) is the refractive index. If the medium is absorbing, then the intensity of the ray decreases and it deposits some power in the domain as it passes through. This is described in greater detail in the section Attenuation Within Domains in Theory for the Geometrical Optics Interface.

A bidirectional coupling between the Geometrical Optics and Heat Transfer interfaces may be required for any of the following reasons:

- The refractive index is temperature dependent.
- The medium undergoes thermal expansion and the refractive index is strain dependent.
- The medium undergoes thermal expansion, causing rays be reflected or refracted at different angles when entering or leaving the medium.

When none of these conditions is met, the Geometrical Optics interface affects the Heat Transfer interface, and a unidirectional coupling is sufficient.

*Heat Source Calculation*

Consider a ray $j$ transferring an amount of power $Q_j$ through a domain. During a small time interval $\Delta t$, the ray propagates a short distance $\Delta s$ from initial position $\mathbf{q}_j$ to position $\mathbf{q}_j + \Delta\mathbf{q}_j$ and its power decreases by an amount $\Delta Q$. Then conservation of energy dictates that the deposited ray power in the domain should increase by $\Delta Q$:

$$Q_{\text{src}}(\mathbf{r}, t + \Delta t) \approx Q_{\text{src}}(\mathbf{r}, t) - \sum_{j=1}^{N} \frac{\partial Q_j}{\partial t} \Delta t \delta(\mathbf{r} - \mathbf{q}_j)$$

where $\delta$ is the Dirac delta function. In the limit as this time derivative becomes arbitrarily small, this expression can be rewritten as

$$\frac{dQ_{\text{src}}}{dt} = -\sum_{j=1}^{N} \frac{\partial Q_j}{\partial t} \delta(\mathbf{r} - \mathbf{q}_j)$$

In this expression, every ray is treated as an infinitesimally small point source. This can lead to numerical issues because the heat source becomes infinitely large at the location of each point source. In the following section an alternative expression for the domain heat source is given.

**CREATING A BOUNDED HEAT SOURCE TERM**

The Ray Heat Source node defines a variable for the contribution to the heat source by rays in each mesh element. This variable uses constant shape functions, so it may be discontinuous across boundaries between elements. For a mesh element $j$ with volume $V_j$ the average heat source $Q_{\text{src},j}$ changes according to the expression

$$\frac{dQ_{\text{src}}}{dt} = -\frac{1}{V_j} \sum_{j=1}^{N} \frac{\partial Q_j}{\partial t} \int \delta(\mathbf{r} - \mathbf{q}_j) dV$$

The integral on the right-hand side is a volume integral over element $j$. The resulting time derivative of the heat source is the average value over the mesh element, which may be written more concisely as

$$\frac{dQ_{\text{src},j}}{dt} = -\frac{1}{V_j} \sum_{i=1}^{N_j} \frac{\partial Q_j}{\partial t}$$

where the sum is taken over all rays that are within mesh element $j$.

# 5

# Glossary

This Glossary of Terms contains modeling terms in a ray optics context. For mathematical terms as well as geometry and CAD terms specific to the COMSOL Multiphysics® software and documentation, see the glossary in the *COMSOL Multiphysics Reference Manual*. For references to more information about a term, see the index.

# Glossary of Terms

**actinometric quantity**  A physical quantity that describes radiative transfer in terms of the number of photons, rather than the total mount of energy.

**blackbody, ideal**  A theoretical surface that absorbs all radiation that is incident upon it, regardless of wavelength or surface temperature.

**blackbody radiation**  Diffuse emission of radiation from the surface of an ideal blackbody.

**coherence**  The degree to which two rays interfere with each other, or to which a ray may interfere with itself when subjected to a time delay.

**cross grating**  A type of diffraction grating with periodicity in two directions.

**diffraction grating**  A periodic structure from which transmitted and reflected radiation can only propagate in specific directions governed by the frequency of radiation and the size of the unit cell.

**diffraction order**  In a diffraction grating, an integer indicating the number of wavelengths between waves emanating from adjacent unit cells before they constructively interfere.

**diffuse emission**  Emission of radiation from a surface in a random direction, following a probability distribution based on Lambert's cosine law.

**diffuse reflection**  Reflection at a surface in a random direction, following a probability distribution based on Lambert's cosine law.

**emissivity, spectral**  The ratio of the amount of radiation per unit surface area, per unit wavelength or frequency, released by an object, compared to an ideal blackbody radiation source of the same size and shape.

**Fresnel equations**  A set of equations for computing the reflection coefficients and transmission coefficients for rays as they cross a boundary between two media with different refractive indices.

**Gaussian beam**  A beam of electromagnetic radiation in which the electric field amplitude follows a Gaussian distribution. In the ideal case, this is the $TEM_{00}$ mode solution to the electromagnetic wave equation in free space.

**geometrical optics**  The analysis of electromagnetic wave propagation through electrically large domains by treating the electromagnetic waves as rays.

**grating**  See **diffraction grating** and **cross grating**.

**graybody radiation**  Diffuse emission from a surface at which the spectral emissivity is constant, independent of wavelength or temperature. Blackbody radiation is the special case for which this constant value of the spectral emissivity is unity.

**intensity**  A measure of the energy density of an electromagnetic wave; for a plane polarized wave, the intensity is equal to the magnitude of the time-averaged Poynting vector.

**internal transmittance**  A material property indicating the fraction of electromagnetic energy that is transmitted through a material sample of a given thickness, neglecting Fresnel losses at the surfaces of the sample. Can be used as an alternative means of specifying the imaginary part of the **refractive index**.

**marginal ray**  The ray that is released from the center of the object at the maximum aperture. This ray will pass through the edge of the aperture stop.

**monochromatic light**  Light of uniform frequency or wavelength.

**Mueller matrix**  A 4-by-4 matrix which can be multiplied by the Stokes vector to apply the effects of various optical components to a ray.

**optical dispersion model**  A function giving the refractive index as a function of wavelength. The coefficients for any given model will usually be determined empirically.

**optical axis**  For simply rotationally symmetric optics, this is the axis of rotational symmetry. The optical axis will pass through the center of curvature.

**optical path length**  The integral of refractive index along the ray trajectory. Over a given time interval, the optical path length of a ray is equal to the distance the ray would have propagated in a vacuum.

**part**  IA subsequence of geometry instructions, usually comprising several geometry primitives, that can be added repeatedly to a COMSOL geometry sequence to avoid repetitive steps in geometry setup.

**phase**  The quantity that indicates the variation of the instantaneous electric field with respect to time and position.

**plane of incidence**  For nonnormal incidence of a ray at a surface, the unique plane containing the surface normal and the incident ray direction vector. For normal incidence, any plane containing the surface normal may be selected.

**photon**  The quantum of the electromagnetic field.

**polarization**  A description of the orientation of the electric field for a polarized or partially polarized ray, and for the way in which this electric field varies as the ray propagates.

**polarization, circular**  The state of polarization in which the electric field amplitude has two orthogonal components of equal magnitude, with a phase shift of $\pi/2$ between them, such that the electric field vector traces a helical pattern as the ray propagates.

**polarization, linear**  The state of polarization in which the electric field only oscillates within a single plane.

**power**  The energy transferred per unit time.

**Poynting vector**  The vector representing the directional energy flux of an electromagnetic field.

**primary ray**  A ray that is released into a model independently of the trajectories of other rays. Primary rays are created by release features.

**principal curvature direction**  A unit vector which, together with the normal to a surface, defines a plane in which one of the principal radii of curvature of a surface is defined.

**polychromatic light**  Light with a distribution of frequencies or wavelengths.

**principal curvature**  The reciprocal of one of the principal radii of curvature of a surface.

**principal radii of curvature**  The maximum and minimum values of the radius of curvature of curves that can be obtained via the intersection of a surface with a plane.

**quasi-monochromatic light**  Light with a distribution of frequencies in which the changes in free-space wavelength are much smaller than the average free-space wavelength.

**radiant exitance, spectral**  The amount of electromagnetic energy emitted from a surface per unit time, per unit surface area, per unit wavelength or frequency.

**radiant exitance, total**  The amount of electromagnetic energy emitted from a surface per unit time, per unit surface area.

**radiometric quantity**  A physical quantity that describes radiative transfer in terms of the amount of energy, including such units as watts, watts per square meter, watts per steradian, and watts per square meter per unit wavelength.

**reflection coefficient**  A dimensionless coefficient that is used to compute the intensity of reflected rays. At boundaries between media, reflection coefficients are computed using the Fresnel equations.

**refractive index**  The ratio of the speed of light in a vacuum to the speed of light in a medium. This is also known as the absolute refractive index.

**refractive index, relative**  The ratio of the absolute refractive index to the refractive index of air.

**release feature**  A feature that releases a predetermined number of rays and assigns initial values to dependent variables associated with the rays.

**secondary ray**  A ray that is produced by the interaction of existing rays with a domain or boundary feature. The degrees of freedom for all secondary rays are preallocated when beginning to run a study.

**Snell's law**  The set of equations that indicates the directions in which reflected and refracted rays will propagate when a ray interacts with a boundary between two media.

**specular reflection**  Idealized reflection at a smooth surface in which the reflected ray lies within the plane of incidence and the angles of incidence and reflection are equal.

**spot diagram**  A type of plot for visualizing the focusing capability of an optical system. It displays the intersection points of rays with a surface, which is often the image plane of the optical system.

**Stokes parameters**  The four Stokes parameters completely characterize the intensity and polarization of a fully polarized, partially polarized, or unpolarized ray. The Stokes parameters can be interpreted as indicators of the ray intensity that would be measured when sending a ray through various arrangements of polarizers and wave retarders.

**thermo-optic dispersion model**  A function giving the change in refractive index as a function of wavelength and temperature.

**transmission coefficient**  A dimensionless coefficient that is used to compute the intensity of refracted rays at boundaries between media. Transmission coefficients are computed using the Fresnel equations.

**wave vector**  A vector in the direction of ray propagation, which indicates the spatial dependence of the instantaneous electric field for coherent radiation.

**wave number**  The magnitude of the wave vector, equal to $\omega/c$, where $\omega$ is the angular frequency and $c$ is the speed of light in the medium.

**wave retarder**  An optical component that applies a phase shift to radiation of a specific polarization with respect to radiation of an orthogonal polarization.

**Zernike polynomial**  A type of polynomial basis that is orthonormal on the unit circle in 2D. Each term comprises a radial component and an azimuthal component, which are multiplied together. The Zernike polynomial basis is used to report optical path differences when interpreting monochromatic optical aberrations.

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