Optical Design with Zemax for PhD - Advanced

Seminar 6 : Physical Modelling IV - Scattering
2015-01-14
Herbert Gross
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2. Surface measurement
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4. Diffraction scattering models
5. Empirical models and BSDF
6. Data of technical surfaces
7. False light in optical systems
8. Calculation of straylight and examples

1. Scattering theory in volumes
2. Exact Maxwell theory
3. Transport theory
4. Diffusion transport
5. Comparison of models
6. Scattering in tissue
7. Examples

1. Scattering in Zemax
basic description of scattering
Different surface geometries:
Every micro-structure generates a specific straylight distribution

- **Smooth surface**
  - Specular reflex
  - No scattering

- **Regular grating**
  - Discrete pattern of diffraction orders

- **Irregular grating**
  - Continuous linear scatter pattern

- **Statistical isotropic surface**
  - Broad scatter spot

Ref.: J. Stover, p.10
Scattering at rough surfaces: statistical distribution of light scattering in the angle domain

Angle indicatrix of scattering:
- peak around the specular angle
- decay of larger angle distributions depends on surface treatment
Definition of Scattering

• Physical reasons for scattering:
  - Interaction of light with matter, excitation of atomic vibration level dipoles
  - Resonant scattering possible, in case of re-emission $\lambda$-shift possible
  - Direction of light is changed in complicated way, polarization-dependent

• Phenomenological description (macroscopic averaged statistics)
  1. Surface scattering:
     1.1 Diffraction at regular structures and boundaries:
         gratings, edges (deterministic: scattering ?)
     1.2 Extended area with statistical distributed micro structures
     1.3 Single micros structure: contamination, imperfections
  2. Volume scattering:
     2.1 Inhomogeneity of refractive index, striae, atmospheric turbulence
     2.2 Ensemble of single scattering centers (inclusions, bubble)

Therefore more general definition:
  - Interaction of light with small scale structures
  - Small scale structures usually statistically distributed (exception: edge, grating)
  - No absorption, wavelength preserved
  - Propagation of light can not be described by simple means (refraction/reflection)
1. Surface scattering
   1.1 Edge diffraction
   1.2 Scattering at topological small structures of a surface
       Continuous transition in macroscopic dimension: ripple due to manufacturing,
       micro roughness, diffraction due to phase differences
   1.3 Scattering at defects (contamination, micro defects), phase and amplitude

2. Scattering at single particles:
   2.1 Rayleigh scattering, \( d << \lambda \)
   2.2 Rayleigh-Debye scattering, \( d < \lambda \)
   2.3 Mie scattering, spherical particles \( d > \lambda \)

3. Volume scattering
   3.1 Scattering at inhomogeneities of the refractive index,
       e.g. atmospheric turbulence, striae
   3.2 Scattering at crystal boundaries (e.g. ceramics)
   3.3 Scattering at statistical distributed dense particles
       e.g. biological tissue
Aspects of Scattering

- Geometry regular - statistical distributed
- Single - multi scattering
- Density of scatterers low - high, independence, saturation, change of illumination
- Near - far field
- Scaling, size of scatterers vs. wavelength, micro - macro
- Coherence, scattering vs. re-emission
- Polarization dependence
- Discret scatterers vs. continuous n-variations
- Absorption
- Diffraction vs. geometrical approach
- Steady state vs time dependence
- Wavelength dispersion of material parameters
- Finite volume size - boundary conditions
Approximations in Scattering Models

- Geometry simplified
- Boundaries simplified, mostly at infinity
- Isotropic scattering characteristic
- Perfect statistics of distributed particles
- Multiple scattering neglected
- Discretization of volume
- Angle dependence of phase function simplified
- Scattering centers independent
- Scatterers point like objects
- Spatially varying material parameters ignored
- Field assumed to be scalar
- Decoherence effects neglected
- Absorption neglected
- Interaction of scatterers neglected
- $\lambda$-dispersion of material data neglected
Available Solutions of Maxwell's Theory

Analytical solutions:
- Spherical particles
  1. generalized Lorentz-Mie theory, near and far field
  2. multi sphere configurations
  3. layered structures
- Spheroids
- Cylinders
  1. single cylinders, with oblique incidence, near and far field
  2. stacked cylinders
  3. multi cylinder configurations, perpendicular incidence

Numerical solutions in time domain:
- Arbitrary geometries
- Finite difference time domain method (FDTD), only small volumes (2\(\mu\)m\(^3\)), \(\Delta x = \lambda/20\)
- Pseudospectral method (PSTD), \(\Delta x = \lambda/4\)

Stationary solutions:
- Discrete dipole approximation for arbitrary geomtries
- T-matrix method

Ref: A. Kienle
Definition of Scattering

- surface measurement
TIS-Measurement with Ulbricht Sphere

- **TIS value (total integrated scattering):**
  total scattered straylight relativ to incoming power

\[ I_{TIS} = \frac{1}{P_i} \cdot \int dP_s = \int_0^{2\pi/2} \int_{0}^{\pi} F_{BSDF}(\theta, \varphi) \cdot \cos \theta \cdot \sin \theta d\theta d\varphi \]

- Measurement of TIS by Ulbricht sphere
- Approximation for small roughness and statistical height distribution for normal incidence

\[ I_{TIS}^{(normal)} = \left( \frac{4\pi \cdot \sigma_{rms}}{\lambda} \right)^2 \]
Measurement of Surface Defects

Distribution into spatial frequency domains

- atomic force microscope
- classical interferometer
- optical heterodyne profilometer
- DIC interference microscope
- mechanical profilometer
- Mirau interferometer
- scattering at 632 nm

Spatial frequency: Log s in 1 / m

Figure: waviness
Waviness: micro roughness

Scales:
- 10^-4 to 10^-1 mm
- 1 to 10 μm
- 10 nm
Fourier description and PSD
Autocorrelation Function

- Autocorrelation function of a rough surface

\[ C(\Delta x) = \langle h(x) \cdot h(x + \Delta x) \rangle = \frac{1}{L} \cdot \int h(x) \cdot h(x + \Delta x) \, dx \]

- Correlation length \( \tau_c \):
  Decay of the correlation function, statistical length scale

- Value at difference zero

\[ C(0) = \sigma_{rms}^2 \]

- Special case of a Gaussian distribution

\[ C(x) = \sigma_{rms}^2 \cdot e^{-\frac{1}{2} \left( \frac{x}{\tau_c} \right)^2} \]
Surface Characterization

\[ h(x) \]

\[ C(\Delta x) = \frac{1}{L} \cdot \int h(x) \cdot h(x + \Delta x) \, dx \]

\[ C(\Delta x) \] autocorrelation

\[ A(k) = \int_0^L h(x, y) \cdot e^{-ikx} \, dx \]

\[ A(k) \] spectrum

\[ F_{PSD}(k) = \frac{1}{L} \cdot \left| \int h(x) \cdot e^{ikx} \, dx \right|^2 \]

\[ F_{PSD}(k) \] power spectral density

< \text{h}_1 \text{h}_2 > \text{ correlation}
PSD of a Surface

- Fourier transform of a surface spectral amplitude density

\[ A(k) = \int_0^L h(x, y) \cdot e^{-ikx} \, dx \]

- PSD power spectral density relative power of frequency components

\[ F_{PSD}(v_x, v_y) = \frac{1}{A} \left| \frac{1}{2\pi} \int \int h(x, y) \cdot e^{2\pi i (x \cdot v_x + y \cdot v_y)} \, dx \, dy \right|^2 \]

- Areae under PSD-curve

\[ \sigma_{rms}^2 = \frac{1}{A} \int \int F_{PSD}(v_x, v_y) \, dv_x \, dv_y \]

\[ v = \frac{1}{D} \ldots \frac{1}{\lambda} \]

- Meaningful range of frequencies

- Polished surfaces are similar and have fractal structure, PSD has slope 1.5 ... 2.5

- Relation to auto-correlation function of the surface

\[ F_{PSD}(v) = \hat{F}[C(x)] = \frac{1}{\pi} \int_0^\infty C(x) \cdot \cos(xv) \, dx \]
Spatial Frequency of Surface Perturbations

- Power spectral density of the perturbation
- Three typical frequency ranges, scaled by diameter $D$
  1. Long range, figure error deterministic description resolution degradation
  2. Mid frequency, critical model description complicated
  3. Micro roughness statistical description decrease of contrast

Limiting line
slope $m = -1.5...-2.5$

$\log A^2_{\text{Four}}$

- Long range, low frequency figure Zernike
- Mid frequency
- Micro roughness

$1/D$ $12/D$ $40/D$ $1/\lambda$
PSD of an Optical Surface

- PSD function, range of spatial frequency:
- Area under curve is proportional to $P_{TIS}$:

$$k = \frac{2\pi}{\lambda} \ldots \frac{2\pi}{\lambda}$$

$$\sigma^2_{rms} = \frac{1}{A} \cdot \int \int F_{PSD}(k) dk \propto P_{TIS}$$

- Typical: limiting straight line, fractal surface
- Wide scale of sizes
- Different measuring tools necessary
Definition of Scattering

- diffraction scattering models
Kirchhoff Theory of Scattering

- Scalar model for straylight calculation with Kirchhoff diffraction integral
  Surface as phase mask

- Approximations:
  - no obscuration
  - smooth surface limit

\[ \frac{\lambda}{8 \cos \theta_i \cdot \sigma_{rms}} \gg 1 \]

\[ E_s(x', y') = E_0 \cdot \int \int e^{2ki\cdot h(x,y)} \cdot e^{\frac{ik}{R}(xx' + yy')} \, dx \, dy \]
Angle distribution in the far field as diffraction integral

\[ E(s_x, s_z) = \int \int e^{\frac{4\pi i}{\lambda} \cos \theta_i \cdot z'(x', y')} \cdot e^{\frac{2\pi i}{\lambda} \cdot f \left( s_x x' \cos \theta_i - s_z z'(x', y') \sin \theta_i + s_y y' \right)} \left( \cos \theta_i - \sin \theta_i \frac{\partial z'}{\partial x'} \right) dx' dy' \]

Special case of sine grating:
- corresponds to one Fourier component
- phase difference \( \Delta \)

\[ z(x) = a \cdot \sin(2\pi s \cdot x + \alpha) \]

\[ P_{scat} = P_0 \cdot \sum_n J_n^2(\Delta) \cdot \cos^2 \theta_n \]
Harvey-Shack Theory

- **Description of scattering by linear system theory**
  \[ \hat{L}_{out} = \hat{H} \cdot \hat{L}_{in} \]
  
  L: ray density

- **Transfer function**
  \[ H_{OTF}^{(S)}(x, y) = e^{-\left(4\pi \cdot \cos \theta_i \cdot \sigma_{rms}\right)^2} \cdot e^{1 - \frac{1}{\sigma_{rms}^2} \cdot C_s \left( \frac{x}{r \cdot r \cdot \cos \theta_i} \right)} \]

- **Angle distribution:**
  1. specular part
  2. scattering part

  \[ L_{PSF}(\alpha, \beta) = \hat{F}[H_S(x, y)] \]
  \[ = A \cdot \delta(\alpha, \beta) + B \cdot S(\alpha, \beta) \]

- **Scattering contribution corresponds to BSDF**

  \[ S(\alpha, \beta) = \frac{I(\alpha, \beta)}{R \cdot P_i \cdot \cos \theta_i} = \frac{1}{R} \cdot F_{BSDF}(\theta_i, \varphi_i, \theta_s, \varphi_s) \]
- BSDF and empirical scattering models
BSDF of a Surface

- Description of scattering characteristic of a surface: BSDF (bidirectional scattering distribution function)

- Straylight power into the solid angle $d\Omega$ from the area element $dA$ relative to the incident power $P_i$

$$F_{BSDF} = \frac{dL_s}{dP_i} = \frac{dP_s}{\cos \theta \cdot dP_i \cdot d\Omega}$$

- The BSDF works as the angle response function

$$P(\theta, \varphi) = \int F_{BSDF}(\theta_i, \varphi_i, \theta, \varphi) \cdot P(\theta_i, \varphi_i) \cdot \cos \theta_i d\Omega_i$$

- Special cases: formulation as convolution integral
BSDF of a Surface

- **3D description of a surface**

- Large angles: consideration of the cosines
  \[
  \alpha = \sin \theta_s \cdot \sin \varphi_s \\
  \beta = \sin \theta_s \cdot \cos \varphi_s - \sin \theta_{\text{spec}}
  \]

- Example distribution

\[
F_{\text{BSDF}} = \begin{cases} 
0 & \text{if } \beta \leq 0 \\
1 & \text{if } \beta > 0 
\end{cases}
\]
- Exponential correlation decay
  PSD is Lorentzian function
  \[ C(x) = \sigma_{rms}^2 \cdot e^{-\frac{x}{\tau_c}} \]
  \[ F_{PSD}(s) = \frac{1}{\pi} \cdot \frac{\sigma_{rms}^2 \cdot \tau_c}{1 + \left(s \cdot \tau_c\right)^2} \]

- Gaussian correlation
  \[ C(x) = \sigma_{rms}^2 \cdot e^{-\frac{1}{2} \left(\frac{x}{\tau_c}\right)^2} \]
  \[ F_{PSD}(s) = \frac{\tau_c \cdot \sigma_{rms}^2}{\sqrt{4\pi}} \cdot e^{\left(-\frac{s\tau_c}{2}\right)^2} \]

- Fractal surface with Hausdorff parameter D
  \[ F_{PSD}(s) = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2\Gamma\left(\frac{1}{2}\right) \cdot \Gamma\left(\frac{n}{2}\right)} \cdot \frac{K_n}{s^{n+1}} \]

- K correlation model parameter B, s
  \[ F_{PSD}(s) = \frac{A}{\left[1 + (s \cdot B)^2\right]^{C/2}} \]
Empirical model function of BSDF

- Notations:
  - Sine of scattering angle: $\sin \theta_s$
  - Slope parameter $m$
  - Glance angle
  - Reference and pivot angle: $\beta_{\text{ref}}$
  - BSDF value at reference: $a$

- Simple isotropic scalar model

F_{BSDF}(\beta) = a \cdot \left( \frac{|\beta - \beta_{\text{spec}}|}{\beta_{\text{ref}}} \right)^m

$\beta = \sin \theta_s$

$\beta_{\text{spec}} = \sin \theta_{\text{spec}}$
Scattering from Optical Surfaces

- Scattering BSDF from polished optical surfaces

\[
BSDF = \frac{2}{\pi} \cdot \frac{(2\pi / \lambda)^4 \cdot \sigma^2 l_c^2}{1 + [2\pi / \lambda \cdot l_c \cdot (\beta - \beta_o)]^2}
\]

\(\sigma\) : rms roughness

\(l_c\) : autocorrelation length

\(\beta - \beta_o\) : scatter angle / deviation

- Increases with nearly \(\lambda^4\)
- Increases with square of surface roughness
- Strong dependence on angle of incidence

Ref: B. Görtlz / Linos
Mirror surface after diamond turning: sinusoidal regular ripple corresponds to radial phase error

Strehl definition for small amplitude $a$ by direct evaluation of the diffraction integral in the far field

$$D_S = \left[ J_0 \left( \frac{2\pi a}{\lambda} \right) \right]^2$$

Shape:
central peak with sidelobes
stronger effect on short wavelength
side lobe energy is related to $a^2$

General approach:
Fourier decomposition of the surface
Harvey-Shack Theory

- Shift invariance around reflection angle
- Symmetric behavior in cos-space

\[ \beta_s - \beta_i \]

\[ \theta_i \]

intensity of straylight

scattering angle

straylight intensity

difference of cosines
Regular Ripple on Diamont Turned Surfaces

- Sinusoidal ripple on mirror surface
  - regular phase perturbation
  - typical from Diamont turning without polishing

- Sinusoidal waveiness with amplitude $a$: Strehl ratio

$$D_s = \left| J_0 \left( \frac{2\pi a}{\lambda} \right) \right|^2$$

- General case:
  Fourier decomposition of the surface topology

- Larger impact on shorter wavelengths
Scattering from Optical Surfaces

- Scattering BSDF from polished optical surfaces

\[
BSDF = \frac{2}{\pi} \cdot \frac{(2\pi / \lambda)^4 \cdot \sigma^2 l_c^2}{1 + [2\pi / \lambda \cdot l_c \cdot (\beta - \beta_o)]^2}
\]

- \( \sigma \): rms roughness
- \( l_c \): autocorrelation length
- \( \beta - \beta_o \): scatter angle / deviation

- Increases with nearly \( \lambda^4 \)
- Increases with square of surface roughness
- Strong dependence on angle of incidence

Ref: B. Görtz / Linos
Scattering from Mechanical Surfaces

- Scattering BRDF from strongly scattering ($\sigma_{\text{rms}} \gg \lambda$) mechanical surfaces

\[
BRDF_{2D} = \pi \cdot R(\theta_i) \cdot F_3^2 \cdot \left( \frac{L}{\lambda} \right)^2 \cdot e^{-fL^2}
\]

\[
L = \frac{\lambda \cdot l_c}{2\pi\sigma (\cos \theta_i + \cos \theta_s)}
\]

\[
F_3 = \frac{1 + \cos \theta_i \cos \theta_s - \sin \theta_i \cos \theta_s \cos \varphi_s}{\cos \theta_i \cdot (\cos \theta_i + \cos \theta_s)}
\]

\[
f = \frac{1}{\lambda} \cdot \sqrt{(\sin \theta_s \cos \varphi_s - \sin \theta_s)^2 + (\sin \theta_s \sin \varphi_s)^2}
\]

$\sigma$ : rms roughness

lc : autocorrelation length

Ref: B. Görtz / Linos
Scattering by Diffraction

- Diffraction scattering BDDF
  
  \[ BDDF(\theta) = \frac{D^2}{\lambda^2} \cdot \left[ \frac{2 \cdot J_1(\pi \cdot D \cdot \sin \theta / \lambda)}{\pi \cdot D \cdot \sin \theta / \lambda} \right]^2 \]
  
  D : diameter of stop

- Approximation of smeared out diffraction rings:
  asymptotic expression

  \[ BDDF(\theta) = \frac{\lambda}{\pi^3 D \cdot \sin \theta} \]

Ref: B. Görtz / Linos
Data of technical surfaces
Roughness of Optical Surfaces

Dependence of treatment technology on roughness

- Grinding
- Polishing
- Computer controlled polishing
- Diamond turning
- Plasma etching
- Magneto-rheological treatment
- Ductile manufacturing
- Ion beam finishing

Roughness rms [nm]

Material removal qmm/s
Roughness of Optical Surfaces

$\lambda$

$\sigma$

super polish

normal polish

metal

$TIS = 10^{-1}$

$TIS = 10^{-2}$

$TIS = 10^{-3}$

$TIS = 10^{-4}$

$TIS = 10^{-5}$

$TIS = 10^{-6}$
Scattering from Optical Surfaces

- Scattering BSDF from polished optical surfaces

\[
BSDF = \frac{2}{\pi} \cdot \frac{(2\pi / \lambda)^4 \cdot \sigma^2 l_c^2}{1 + [2\pi / \lambda \cdot l_c \cdot (\beta - \beta_o)]^2}
\]

- \(\sigma\): rms roughness
- \(l_c\): autocorrelation length
- \(\beta - \beta_o\): scatter angle / deviation

- Increases with nearly \(\lambda^4\)
- Increases with square of surface roughness
- Strong dependence on angle of incidence

Ref: B. Görtz / Linos
Measurement of BRDF measurement incidence / observation angle

Ref: A. Bodemann

Lastina

Institute of Applied Physics
Friedrich-Schiller-Universität Jena
Measurement of BRDF functions

Ref: A. Bodemann
Measurement of BRDF functions

From: A. Bodemann
- Maximum BRDF at angle of reflection
- Larger BRDF for skew incidence

Ref.: A. Bodemann
- Logarithmic scale in value and angle distance to specular case
Scattering BSDF Decomposition

- Bidirectional scattering distribution function
- Decomposition into three types
- Several reasons for scattering
- BSDF is additive

\[ BSDF_{surf}(\theta, \varphi) = \sum_j BSDF_j(\theta, \varphi) \]

Ref: B. Görtz / Linos

BSDF (scattering)

BRDF (reflection)

BRTF (transmission)

BDDF (diffraction)

roughness
surface defects
particle contamination
coating irregularities

Ref: B. Görtz / Linos
Particles on Optical Surfaces

- Model of Mie scattering at particle contamination

Ref: B. Götz / Linos
Particles on Optical Surfaces

- Cleaned surface

Ref: B. Görtz / Linos

- Size of particles in μm
- Number of particles

Cleaned surface
dark field microscopic image

Ref: B. Görtz / Linos
false light in optical systems
Sources of Stray Light

1. Direct imaging ray path

2. Direct reflected ray (zero order false light)
   - Reflected from optical surface
   - Reflected by mechanical parts

3. Scattered light
   - Scattered on surface micro structure
     - Optical surface
     - Mechanical surface
   - Scattered on particles
   - Volume scattering

4. Diffraction
   - Apertures and baffles

Ref: B. Goerz
Ghost Images

Ghost image in photographic lenses:
Reflex film / surface

Ref: K. Uhlendorf, D. Gängler
Straylight and Ghost Images

- Different reasons
- Various distributions
Scattering of Light

- Scattering of light in diffuse media like frog

Ref: W. Osten
Straylight and Ghost Images

- Calculation of reflected light
- Colour effects due to coatings

Ref.: M. Peschka
Calculation of straylight and examples
- Photometrical calculation of the transfer of energy density

\[ dP = L \cdot \cos \theta \cdot dA \cdot d\Omega \]

- Integration of the solid angle by raytrace

- In the system model

\[ P = E_s \cdot g \cdot T \cdot F_{BRDF} \cdot \Omega \]

g : geometry factor

surface response : BSDF

T : transmission

Practical Calculation of Straylight

incident ray

mirror

next surface

real used solid angle

\( F_{BRDF} \)
Practical Calculation of Straylight

- Decomposition of the system into different ray paths

- Properties:
  - extrem large computational effort
  - important sampling guarantees quantitative results for large dynamic ranges
  - mechanical data necessary and important
    - often complicated geometry and not compatible with optical modelling
  - surface behavior (BRDF) necessary with large accuracy
- Optimal design of straylight suppressing diaphragms
- Design and geometry of baffle diaphragms

- Baffle Design

- comfortable

- better

- uncomfortable

- incident direction of secondary light source

- no direct reflected light into signal direction

- double reflected

- further optical system
Suppression of Straylight

- Clever geometry of lens boundary
- Appropriate coatings with reflectivity $r$ on surfaces
- Provoke $n$-times multiple scattering events with lower probability

$R_{ges}$

$r$ decreased

$n$ increased

$n = 1$

$n = 2$

$n = 3$

$n = 4$

$n = 5$
1. Mechanical system

2. Simplified mechanics

3. Critical straylight paths

Ref: R. Sand
Straylight at Mechanical Parts

Selection of the relevant parts of a full CAD mechanical model
- Straylight calculation in a telescope
- Contributions form:
  1. surfaces
  2. mechanical parts
  3. diffraction at edges

Example for Straylight in a Telescope

\[
\log I(q) = 10^{-5}, 10^{-7}, 10^{-9}
\]

- collimator
- spider
diffraction
primary mirror
secondary mirror
aperture diffraction

\[ \theta \]
Scattering Theory in volumes
Model Options

- 3 major approaches
- Analytical vs. numerical solutions

Diagram:

- Rigorous Maxwell solutions
  - Analytical (Mie spheres, Cylinders)
  - Numerical (T-matrix, PSTD, FDTD, GLMT)

- Radiation transport equation
  - Analytical (spheres)
  - Numerical (FD-grid-based, Monte Carlo, SH expansion, Finite elements)
  - Features: polarization (PMC), electric field (EMC), particles fixed, time resolved

- Diffusion equation
  - Analytical (bricks)
  - Numerical (FD-grid based, FE, layered, cylinder)
Model Validity Ranges

- Typical tissue features
- Model validity ranges

- Cell membranes
- Macromolecule aggregates, stiations in collagen fibrils
- Mitochondria
- Vesicles, lysosomes
- Cell nuclei
- Cells

Typical scale size $\lambda = d$

- Single: Rayleigh
- Single: Mie
- Volume: Maxwell
- Volume: RTE
The Volume Dilemma

- **Problem:**
  - Exact solutions of scattering: Maxwell equations
  - volume sampling requires large memory
  - realistic simulations: small volumes (2 \(\mu\)m\(^3\))
  - real sample volumes can not be calculated directly

- **Approach:**
  - Calculation of response function of microscopic scattering particles with Maxwell equations
  - empiricial approximation of scattering phase function \(p(\theta,\varphi)\)
  - solution of transport theory with approximated scattering function

Ref: A. Kienle
Model Validity Ranges

- Simple view: diagram volume vs. density
- Transition form single scatterers to extended volumes
- Sample types are essential
- Approximations are necessary

---

**Aggregation to Extended Samples**

- **Single particles**
  - Rayleigh
  - Spheres: Mie
  - Cylinders
  - Maxwell FDTD
  - Maxwell PSTD
  - Maxwell T-matrix
  - Maxwell Multipol expansion

- **Aggregates of single particles**
  - Spheres: multiple Mie
  - Multiple Cylinders
  - Maxwell PSTD
  - Maxwell T-matrix
  - Maxwell Multipol expansion

- **Dense media resolved into single particles (with interaction)**
  - Single scattering particles
    - exact
    - Aggregation in RTE approximation

- **Dense media with continuous random index distribution**
  - Beam propagation
  - RTE approximation
  - Diffusion approximation
Scattering Theories

- Approximations and assumptions:
  1. low density, no interaction of scatter events
  2. no absorption
  3. statistical distribution of many isolated small scatter centers

- Approach: description with BSDF function
  \( C_s \) cross section area
  \( \rho_s \) density
  \( p(\theta) \) phase function

\[
F_{BSDF} = \frac{1}{4\pi \cdot \cos \theta_i \cos \theta_s} \cdot C_s \cdot p(\theta) \cdot \rho_s
\]
Exact Maxwell Theory
Available Solutions Maxwell Theory

Analytical solutions:
- Spherical particles
  1. generalized Lorentz-Mie theory, near and far field
  2. multi sphere configurations
  3. layered structures
- Spheroids
- Cylinders
  1. single cylinders, with oblique incidence, near and far field
  2. stacked cylinders
  3. multi cylinder configurations, perpendicular incidence

Numerical solutions in time domain:
- Arbitrary geometries
- Finite difference time domain method (FDTD), only small volumes (2μm^3), Δx = λ/20
- Pseudospectral method (PSTD), Δx = λ/4

Stationary solutions:
- Discrete dipole approximation for arbitrary geometries
- T-matrix method

Ref: A. Kienle
Rigorous Scattering at Sphere

- Maxwell solution in the nearfield

\[ \lambda = 600 \text{ nm} \quad n_{\text{out}} = 1.33 / n_{\text{in}} = 1.59 \quad n_{\text{out}} = 1.59 / n_{\text{in}} = 1.33 \quad n_{\text{out}} = 1.33 / n_{\text{in}} = 1.59 + 5i \]

- \( r = 1 \mu m \)
- \( r = 2 \mu m \)

Ref: J. Schäfer
Multiple Scattering

- Change of scattering cross section due to shadowing effects
- Phase function depends on neighboring particle

Ref: J. Schäfer
Aggregation to Extended Samples

- Larger aggregates of simple single scatter particles
- Can be treated rigorous for moderate numbers/volumes
Rayleigh-Scattering

- Scattering at particles much smaller than the wavelength
  \[ d \ll \lambda \]

- Scattering efficiency decreases with growing wavelength
  \[ Q_s = \frac{128\pi^4 a^4}{3\lambda^4} \left| \frac{n_s^2 - n^2}{n_s^2 + 2n^2} \right| \]

- Angle characteristic depends on wavelength
- Phase function
  \[ p(\theta) = \frac{3}{16\pi} \cdot (1 + \cos^2 \theta) \]

- Example: blue color of the sky
Mie Scattering

- Result of Maxwell equations for spherical dielectric particles, valid for all scales
- Interesting for larger sizes \( d \gg \lambda \)

- Macroscopic interaction:
  - Interference of partial waves,
  - Complicated angle distribution
- Usually dominating: forward scattering
- Parameter: \( n, n', d, \lambda, (\alpha) \)
- Example: small water droplets (\( d=10 \, \mu m \))
- Limitation: interaction of neighboring particles

- Approximation of parameter
  \[
  5\lambda < 2\pi \cdot n \cdot a < 50\lambda \quad \text{and} \quad n < n_s < 1.1n
  \]

Cross section

\[
\sigma = 3.28 \cdot \left( \frac{2\pi nd}{\lambda} \right)^{0.37} \left( \frac{n'}{n} - 1 \right)^{2.09}
\]

Ref.: M. Möller
Mie Scattering Phase Function

- Shape of the phase function due to Mie scattering:
  - growing complexity with radius of sphere
  - interference condition complicated
  with several points of stationary phase

Ref: J. Schäfer
Transport Theory
Radiative transport equation: photon density model (gold standard for large volumes),
Purely energetic approach, no diffraction
Integration of PDE by raytracing or expansion in spherical harmonics
Options:
1. time, space and frequency domain
2. fluorescence
3. polarization
4. flexible incorporation of boundaries and surfaces, voxel based
Analytical solutions for special geometries:
1. several source geometries
2. space extended to infinity
3. Already some minor differences to Monte-Carlo approach due to assumptions
Not included features:
1. diffraction, no description of speckles, interference
2. no coherent back scattering
3. no dependencies of neighboring scatterers
Radiance Transport Equation

- Description of the light propagation with radiance transport equation for photon density balance:
  1. incoming photons
  2. outgoing photons
  3. absorption, extinction
  4. emission, source

\[
\frac{1}{c} \frac{\partial L(\vec{r}, t, \vec{s})}{\partial t} + \vec{s} \cdot \nabla L(\vec{r}, t, \vec{s}) + (\mu_a + \mu_s) \cdot L(\vec{r}, t, \vec{s}) = \mu_s \cdot \int L(\vec{r}, t, \vec{s}) \cdot p(\vec{s}, \vec{s'}) \, d\omega + Q(\vec{r}, t, \vec{s})
\]

- Numerical solution approach:
  Expansion into spherical harmonics
Diffusion Theory
Diffuse Light Propagation: General Model

- General radiation transfer equation (RTE, Boltzmann)

\[
\frac{1}{c} \frac{\partial L(\vec{r}, t, \vec{s})}{\partial t} + \vec{s} \cdot \nabla L(\vec{r}, t, \vec{s}) + (\mu_a + \mu_s) \cdot L(\vec{r}, t, \vec{s}) = \mu_s \cdot \int L(\vec{r}, t, \vec{s'}) \cdot p(\vec{s}, \vec{s'}) d\omega + Q(\vec{r}, t, \vec{s})
\]

- Local balance of photon numbers:
  1. Incoming photons, divergence
  2. Outgoing photons, scattering
  3. Absorbed photons, extinction
  4. Emitted photons, source

- Problem: direction dependence of scattering

- Approximative phase function \( p \) of the scattering process: Henyey-Greenstein
  \( g \) : mean of scattering anisotropy

\[
p_{HG}(\vec{s}, \vec{s'}) = \frac{1}{4\pi} \cdot \frac{1 - g^2}{\left[1 + g^2 - 2g\vec{s} \cdot \vec{s'}\right]^{3/2}}
\]
Severe approximations assumed:
- perfect isotropic scattering
- no wave optical effects
- description of light as photon density evolution

Time dependent or steady state

Analytical solutions for special geometries
1. Infinity
2. semi-infinity
3. bricks
4. Layered structures
5. cylinder
6. Spheres
Diffusion Equation

- Approximation:
  - scattering dominates gradient effects
  - scattering interaction is isotropic

- Radiance:

- Diffusion equation

- Isotropic diffusion constant

- Mean free path

- Stationary and isotropic
Scattering Theory Comparisons
Modelling Fluorescence

- Models:
  1. Maxwell theory simulation
  2. Monte Carlo calculation
  3. Diffusion theory
- Different approaches
- Under investigation

Ref: A. Kienle
Comparison of Methods

- Analytical solutions with Maxwell solver
  Multiple cylinder geometry

- RTE with Maxwell analytic
  Multiple spheres

Ref: A. Kienle
Comparison of Methods

- RTE with Maxwell analytic with polarization
  Multiple spheres

Ref: A. Kienle
Comparison of Methods

- RTE with Maxwell numeric
  Multiple spheres

Ref: J. Schäfer
Comparison of Methods

- Diffusion versus Monte Carlo method
  Spatial domain

- Diffusion versus Monte Carlo method
  Time domain

Ref: A. Kienle
Scattering in Tissue
Henyey-Greenstein Scattering Model

- Henyey-Greenstein model for human tissue
  Phase function

- Asymmetry parameter $g$:
  Relates forward / backward scattering
  $g = 0$ : isotropic
  $g = 1$ : only forward
  $g = -1$: only backward

- Rms value of angle spreading

$$\theta_{rms} = \sqrt{2(1-g)}$$

- Typical for human tissue:
  $g = 0.7 ... 0.9$

$$p_{HG}(\theta, g) = \frac{1}{4\pi} \cdot \frac{1 - g^2}{\left(1 + g^2 - 2g \cos \theta\right)^{3/2}}$$

$$g = \langle \cos \theta \rangle = \int p(\theta) \cos \theta \, d(\cos \theta) = 2\pi \int_0^\pi p(\theta) \cos \theta \sin \theta \, d\theta$$
Henyey-Greenstein Model

- Simple model for phase function in the case of scattering in biological tissue:

- Values for human tissue

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<th>λ</th>
<th>μs [mm⁻¹]</th>
<th>μs [mm⁻¹]</th>
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Log p

\[
\log p
\]

\[
\text{g = 0, isotrop}
\]

\[
g = 0.3
\]

\[
g = 0.5
\]

\[
g = 0.7
\]

\[
g = 0.95
\]
Henyey-Greenstein Model

- Extended representation 1:
  superposition of two terms

\[
p_{DHG}(\theta, a, g_1, g_2) = a \cdot \frac{1}{4\pi} \cdot \frac{1 - g_1^2}{\left(1 + g_1^2 - 2g_1 \cos \theta \right)^{3/2}} + (1 - a) \cdot \frac{1}{4\pi} \cdot \frac{1 - g_2^2}{\left(1 + g_2^2 - 2g_2 \cos \theta \right)^{3/2}}
\]

\[
= a \cdot p_{HG}(\theta, g_1) + (1 - a) \cdot p_{HG}(\theta, g_2)
\]

- Extended representation 2:
  Two parameters
  More realistic

\[
p_{CS}(\theta, g) = \frac{3}{2} \cdot \frac{1 - g^2}{2 + g^2} \cdot \frac{1 + \cos^2 \theta}{\left(1 + g^2 - 2g \cos \theta \right)^{3/2}}
\]
LSM-Simulation: Cell Model

- cell model after Starosta & Dunn (3D Computation of Focused Beam Propagation through Multiple Biological Cells, OE 17, 12455, 2009)
  - cell: ellipsoid with $n = 1.36$
  - nucleus: sphere with $n = 1.4$
  - 100 mitochondria: ellipsoids with $n = 1.4$
  - 4 fluorescence beads (zero Stokes-shifts)

Ref: S. Siegler
Real Scatter Objects

Bio-medical real sample examples

cancer cell
dentin
cell complex

blood vessel
muscle fibers
wood
Approaches of Biological Straylight Simulation

- Large scale / cells: macroscopic range
  - Diffusion equation, isotropic
  - Some analytical solutions, numerical with spherical harmonics expansion
  - Parameters: effective $\mu'_s$, $\mu_a$, n

- Medium scale / cell fine structure:
  - Mesoscopic range
  - Transport theory, radiation propagation
  - Only numerical solutions, scalar anisotropic
  - Preferred: Monte-Carlo raytrace
  - Some analytical solutions
  - Parameters: $\mu_s, \mu_a, n, p(\phi, \theta)$

- Fine scale: microscopic range
  - Only small volumes, with polarization
  - Maxwell equation solver, FDTD, PSTD
  - Some analytical solutions
  - Parameter: complex index $n(r)$

- Correct scaling: feature size vs. wavelength, depends on application
Scattering in Tissue

- Scattering in biological tissue: Relevant for therapeutic spectral window $\lambda = 650 \text{ nm}...1.3 \text{ mm}$

- Definition / typical numbers:
  - coefficient of absorption: $\mu_a \approx 0.01 ... 1 \text{ mm}^{-1}$
  - coefficient of scattering: $\mu_s \approx 10 ... 100 \text{ mm}^{-1}$
    dominating: scattering with forward direction
  - total attenuation of ballistic photons $\mu_t = \mu_a + \mu_s$
  - Albedo (scattering contribution on attenuation) $a = \mu_s / \mu_t \approx 0.99 ... 0.999$
  - mean free path of photons $s = 1 / \mu_s \approx 10 ... 100 \mu\text{m}$

Ref.: M. Möller
Scattering in Tissue

- **Best approximation depends on ratio** $\mu_s' / \mu_a$ ab ($\mu_s'$: forward scattering)
  - $\mu_a >> \mu_s'$: Lambert-Beer law ($\lambda < 300$nm, $\lambda > 2000$nm)
  - $\mu_a << \mu_s'$: Diffusion approximation (650nm < $\lambda$ < 1150nm)
  - $\mu_a \approx \mu_s'$: RTE equation, Monte-Carlo-simulations
    (300nm < $\lambda$ < 650nm, 1150nm < $\lambda$ < 2000nm)

- **In therapeutic window:**
  Diffusion approximation is good,
  equivalent scattering coefficient

  $$\mu_{eff} = \sqrt{3\mu_a (\mu_a + \mu_s')}$$

  penetration depth

  $$\delta = \frac{1}{\sqrt{3\mu_a (\mu_a + \mu_s')}} \approx 1\ldots 5\text{mm}$$

  Diffusion constant

  $$D = \frac{1}{3(\mu_a + \mu_s')}$$

Ref.: M. Möller
Modelling Light Scattering in Tissue: Backscattering

- Processes

- Simulation

Ref: A. Kienle
Examples
Application: OCT

- Optical coherence tomography:
- Backscattering of light with broad spectrum.
- Depth discrimination by axial coherence length
- Generation of 3D images in tissue

Example:
Image of fundus
Light Scattering in Beer

- The absorption in beer is dispersive
- A longer path length changes the spectral composition of white light illumination
- Daylight illumination from the side gives the characteristic color
- Illumination from the bottom changes the color from yellow to red depending on the height

Ref: A. Kienle
Modelling of Volume Scattering

- Calculation:
  1. Geometrical approximation:
     Raytrace with Monte-Carlo-method
time consuming, non-smooth results

  2. Wave optical with beam propagation
     Scalar approach only for large scales

  3. Diffusion theory:
     In strongly scattering media with isotropic behavior; tissue
Scattering in Zemax
Scattering in Zemax

- Definition of scattering at every surface in the surface properties of sequential mode

- Possible options:
  1. Lambertian scattering indicatrix
  2. Gaussian scattering function
  3. ABg scattering function
  4. BSDF scattering function (table)
  5. User defined

- More complex problems only make sense in the non-sequential mode of Zemax, here also non-optical surfaces (mechanics) can be included

- Surface and volume scattering possible

- Optional ray-splitting possible

- Relative fraction of scattering light can be specified
Definition of scattering at every surface in the surface properties of non-sequential mode

Options:
1. Scatter model
2. Surface list for important sampling
3. Bulk scattering parameters
Definition of scattering at a surface in the non-sequential mode
1. selection of scatter model
2. for some models:
   - to be fixed:
     - fraction of scattering
     - parameter $\sigma$
     - number of scattered rays for ray splitting
Scattering Functions in Zemax

- Surface scattering:
  Projection of the scattered ray on the surface, difference to the specular ray: $x$

- Lambertian scattering:
  isotropic

- Gaussian scattering

- ABg model scatter

- BSDF by table

- Volume scattering: Angle scattering description by probability $P$

- Henyey-Greenstein volume scattering
  (biological tissue model)

- Rayleigh scattering

\[
F_{BSDF}(x) = A
\]

\[
F_{BSDF}(x) = A \cdot e^{-\frac{|x|^2}{\sigma^2}}
\]

\[
F_{BSDF}(x) = \frac{A}{B + |x|^g}
\]

\[
P(\theta) = \frac{1 - g^2}{4\pi \cdot \left(1 + g^2 - 2g \cos \theta\right)^{3/2}}
\]

\[
P(\theta) = \frac{3}{8\lambda^4} \cdot \left(1 + \cos^2 \theta\right)
\]
### Scattering Tables in Zemax

- Data file with scattering functions: ABg-data.dat
- File can be edited

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Scattering Input and Viewing in Zemax

- Tools / Scatter / ABg Scatter Data Catalogs
- Specification and definition of scattering parameters for a new ABg-modell function: wavelength, angle, A, B, g
- Analysis / Scatter viewers / Scatter Function Viewer
  Graphical representation of the scattering function
Scattering with Importance Sampling

- Acceleration of computational speed:
  1. scatter to - option, simple
  2. Importance sampling with energy normalization

- Importance sampling:
  - fixation of a sequence of objects of interest
  - only desired directions of rays are considered
  - re-scaling of the considered solid angle
  - per scattering object a maximum of 6 target spheres can be defined
- Definition of bulk scattering at the surface menue
- Wavelength shift for fluorescence is possible
- Typically angle scattering is assumed
- Some DLL-model functions are supported:
  1. Mie
  2. Rayleigh
  3. Henyey-Greenstein
Scattering Example I

- Simple example: single focussing lens
- Gaussian scattering characteristic at one surface
- Geometrical imaging of a bar pattern
- Image with / without Scattering
  Scattering must be activated in settings
- Blurring increases with growing $\sigma$-value
Scattering Example II

- Example from samples with non-sequential mode
- Important sampling accelerates the calculation
Scattering Bulk Example

- Volume scattering example
- Stokes shift is possible for fluorescence