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Preparatory School to the Winter College on Optics: Advances in Nano-Optics and Plasmonics

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Some Modelling and Calculation Methods for Micro and Nano Optics

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Some Modelling and Calculation Methods for Micro and Nano Optics

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Preparatory School to the Winter College on Optics: Advances in Nano-Optics and Plasmonics, Trieste - Italy, 30 January 2012 - 3 February 2012

Outline

- Stratified media
  – *matrix formalism*
- Stratified media with arbitrary (periodic) profiles
  – *C-method*
- Single Objects
  -*Boundary Element Method (BEM)*
- Complex Objects
  - *Finite Element Methods (FEM)*

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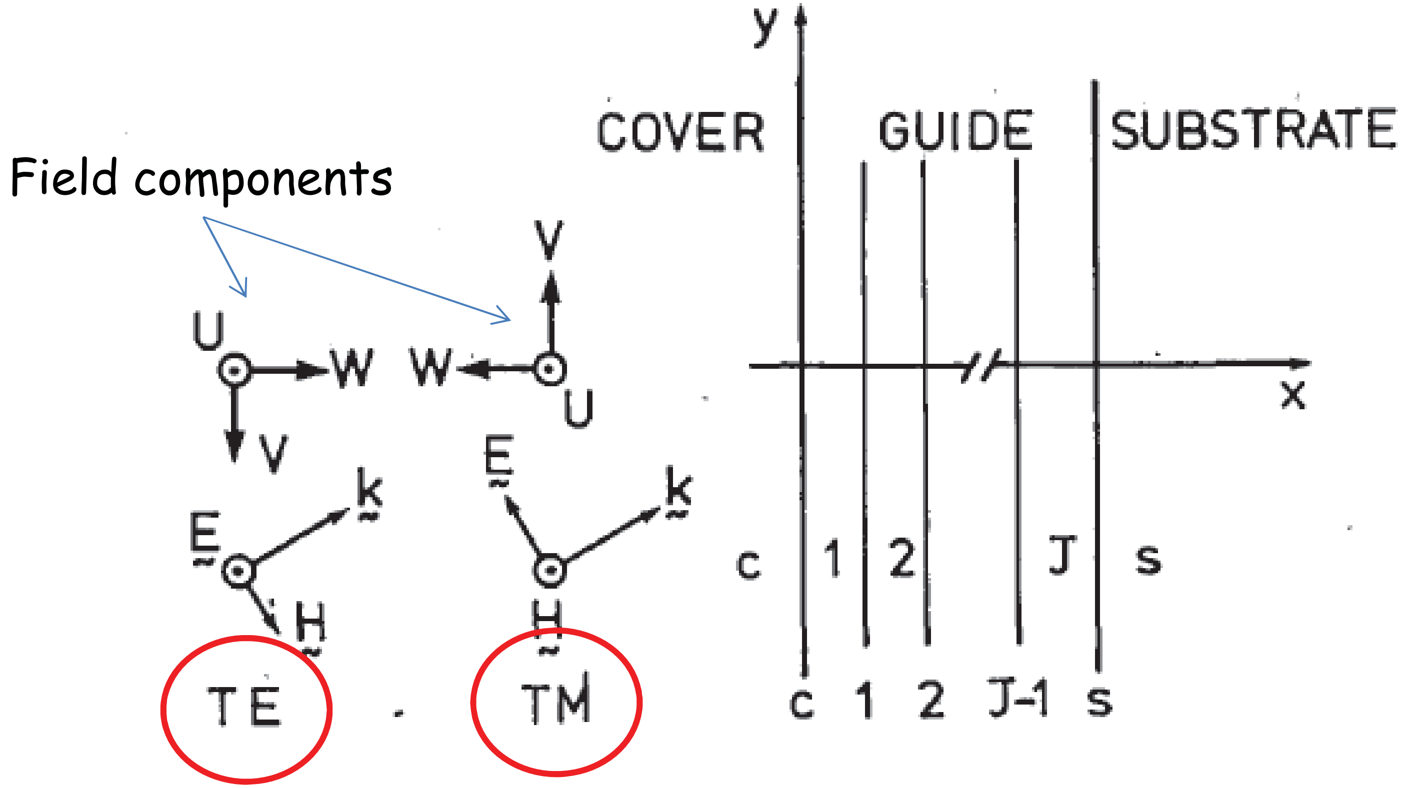
Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A 1,742 (1984)

Steady-state solutions to Maxwell Eq. after imposing boundary conditions



Other polarization states can be obtained as linear combinations of TE and TM

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A 1,742 (1984)

In the International System of Units, the magnitudes of the electric and magnetic fields of a plane electromagnetic wave traveling in a nonmagnetic medium of refractive index n are related by

$$H = \frac{nE}{z_0}, \qquad (1)$$

where $z_0 = (\mu_0/\varepsilon_0)^{1/2}$ is the impedance of free space. The two polarizations are distinguished by the parameter ρ:

$$\rho = \begin{cases} 0 & \text{TE} \\ 1 & \text{TM} \end{cases}, \qquad (2)$$

and the waves have temporal and spatial dependence $\exp[ik(\pm\alpha x + \beta y) - i\omega t]$, where propagation in the positive y direction has been assumed.

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A **1**,742 (1984)

We denote the angle of incidence by θ, and α and β are direction cosines in the positive quadrant multiplied by the refractive index; thus

$$\alpha = n \cos\theta = (n^2 - \beta^2)^{1/2}, \tag{3}$$

$$\beta = n \sin\theta. \tag{4}$$

According to both Snell's law and the law of reflection, β has the same value in all media and is termed the propagation constant or, in the case of guided modes, the effective index (of refraction).

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A 1,742 (1984)

By considering the sum of positive- and negative-going waves at a point in the multilayer, it is evident that the components of the total electric- and magnetic-field vectors have the general form of a plane wave propagating along the positive y axis with nonuniform amplitude $f(x)\exp(ik\beta y - i\omega t)$. For each polarization, three of the field components are zero, and the amplitudes of the nonzero components are assigned to U, V, and W according to Table 1.

BLOCH WAVES

Table 1. Polarization-Dependent Parameters ρ and γ and Field Amplitudes U, V, and W[a]

Polarization	ρ	γ	U	V	W	Remaining Field Components
TE	0	α/z_0	E_z	$-H_y$	H_x	$H_z = E_y = E_x = 0$
TM	1	$\alpha z_0/n^2$	H_z	E_y	$-E_x$	$E_z = H_y = H_x = 0$

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A **1**,742 (1984)

The parameter γ, defined as $\alpha/c\mu$ for the TE polarization and $\alpha/c\varepsilon$ for the TM polarization, becomes, in nonmagnetic media,

$$\gamma = \begin{cases} n \cos\theta/z_0 & \text{TE} \\ z_0 \cos\theta/n & \text{TM} \end{cases}. \quad (5)$$

According to Maxwell's equations, the amplitudes of the field components are related by

$$V = \frac{\gamma}{ik\alpha}\frac{\mathrm{d}U}{\mathrm{d}x}, \quad (6a)$$

$$W = \frac{\beta\gamma}{\alpha}U, \quad (6b)$$

$$U = \frac{1}{ik\gamma\alpha}\frac{\mathrm{d}V}{\mathrm{d}x}. \quad (6c)$$

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A **1**,742 (1984)

The tangential field components U and V are continuous across the interfaces, whereas W is the amplitude of the component normal to the interfaces and is proportional to U. Therefore a total field is adequately specified by the vector $\binom{U}{V}$. A positive-going traveling wave is distinguished from the total field by use of the notation U^+, etc. and is represented by

$$\begin{pmatrix} U^+ \\ V^+ \end{pmatrix} = \begin{pmatrix} 1 \\ \gamma \end{pmatrix} U^+, \tag{7}$$

whereas negative-going waves are distinguished by a negative superscript:

$$\begin{pmatrix} U^- \\ V^- \end{pmatrix} = \begin{pmatrix} 1 \\ -\gamma \end{pmatrix} U^-. \tag{8}$$

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A **1**,742 (1984)

A unimodular field-transfer matrix M_j relates the field amplitudes U_j and V_j at x_j to the corresponding amplitudes at a second point x_{j-1}:

$$\begin{pmatrix} U_{j-1} \\ V_{j-1} \end{pmatrix} = M_j \begin{pmatrix} U_j \\ V_j \end{pmatrix}. \tag{9}$$

The form of the matrix M_j can be readily derived by expressing U and V in terms of positive- and negative-going traveling fields. The result is

$$M_j = \begin{pmatrix} \cos\Phi_j & \dfrac{-i}{\gamma_j}\sin\Phi_j \\ -i\gamma_j \sin\Phi_j & \cos\Phi_j \end{pmatrix}, \tag{10}$$

where $\Phi_j = k\alpha_j(x_j - x_{j-1})$ is the phase thickness of the layer.

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A **1**,742 (1984)

The transfer matrix for a stack consisting of J films is given by the product of the respective transfer matrices for the individual layers:

$$M = \prod_{j=1}^{J} M_j. \tag{11}$$

When the propagation constant β is real and the media are nondissipative dielectrics (real refractive indexes), the diagonal elements m_{11} and m_{22} of the transfer matrix are real, whereas the off-diagonal elements m_{12} and m_{21} are imaginary.

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A 1,742 (1984)

Suppose a plane wave in the cover is incident on the stack; then expressions for the reflection and transmission coefficients (r and t) and intensities (R and T) are readily derived by relating the amplitudes of the incident, reflected, and transmitted traveling-wave fields to the amplitudes U and V of the components of the total fields. By defining $r_{cs} = U_c^-/U_c^+$ as the ratio of the reflected and incident parts of U_c and $t_{cs} = U_s^+/U_c^+$ as the ratio of U_s and the incident part of U_c, we obtain the matrix equation

$$\begin{pmatrix} 1 + r_{cs} \\ \gamma_c(1 - r_{cs}) \end{pmatrix} = M \begin{pmatrix} 1 \\ \gamma_s \end{pmatrix} t_{cs}. \quad (12)$$

By solving the equations for r_{cs} and t_{cs} we obtain

$$r_{cs} = \frac{\gamma_c m_{11} + \gamma_c \gamma_s m_{12} - m_{21} - \gamma_s m_{22}}{\gamma_c m_{11} + \gamma_c \gamma_s m_{12} + m_{21} + \gamma_s m_{22}}, \quad (13)$$

$$t_{cs} = \frac{2\gamma_c}{\gamma_c m_{11} + \gamma_c \gamma_s m_{12} + m_{21} + \gamma_s m_{22}}. \quad (14)$$

Stratified media – *matrix formalism*

J. Chilwell and I. Hodgkinson, J. Opt. Soc. Am. A 1,742 (1984)

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$$\begin{pmatrix} 1 + r_{cs} \\ \gamma_c(1 - r_{cs}) \end{pmatrix} = M \begin{pmatrix} 1 \\ \gamma_s \end{pmatrix} t_{cs}. \tag{12}$$

we obtain

$$R = |r|^2,$$

$$T = \frac{\mathrm{Re}(\gamma_s)}{\mathrm{Re}(\gamma_c)} |t|^2$$

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Stratified media with arbitrary profiles

__Chandezon Method (C-method):__

- Fourier-based method connecting the harmonic components of periodic interfaces to diffraction orders (propagative and evanescent) of output light

- Coordinate-tranformations

- see attached .pdf file with complete description and rigorous derivation

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Single Objects – Boundary Element Method

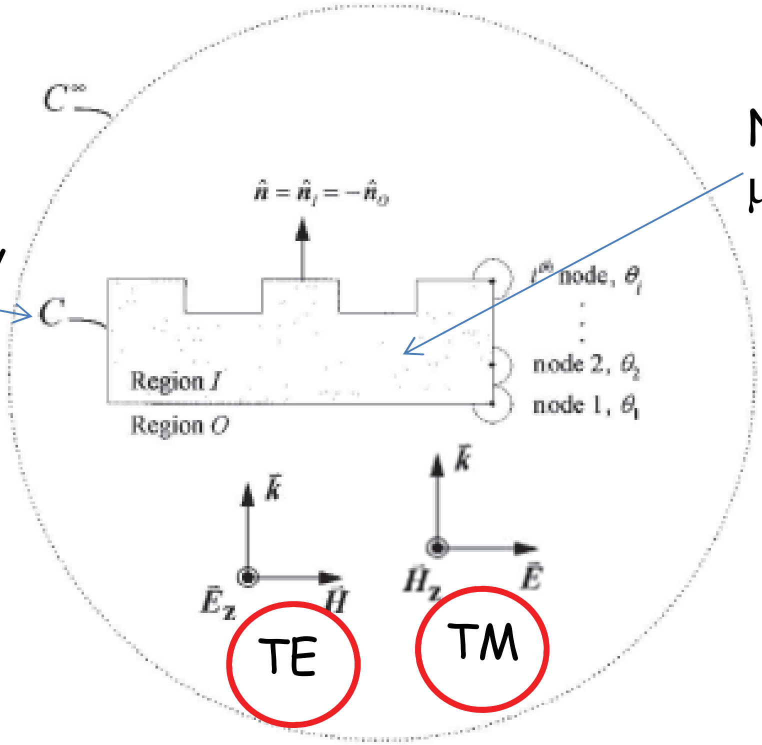
D. W. Prather et al., J. Opt. Soc. Am. A **14**, 34 (1997)

<u>BEM Method</u>

Integral method for solving Maxwell (Helmholtz) equations for TE and TM polarizations

Object boundary

Non-magnetic object:
$\mu_r=1$



$u^{tot}(\mathbf{r})=u^{inc}(\mathbf{r})+u^{sc}(\mathbf{r})$

$u(\mathbf{r})=E_z$ for TE

$u(\mathbf{r})=H_z$ for TM

Single Objects – Boundary Element Method

D. W. Prather et al., J. Opt. Soc. Am. A **14**, 34 (1997)

BEM Method

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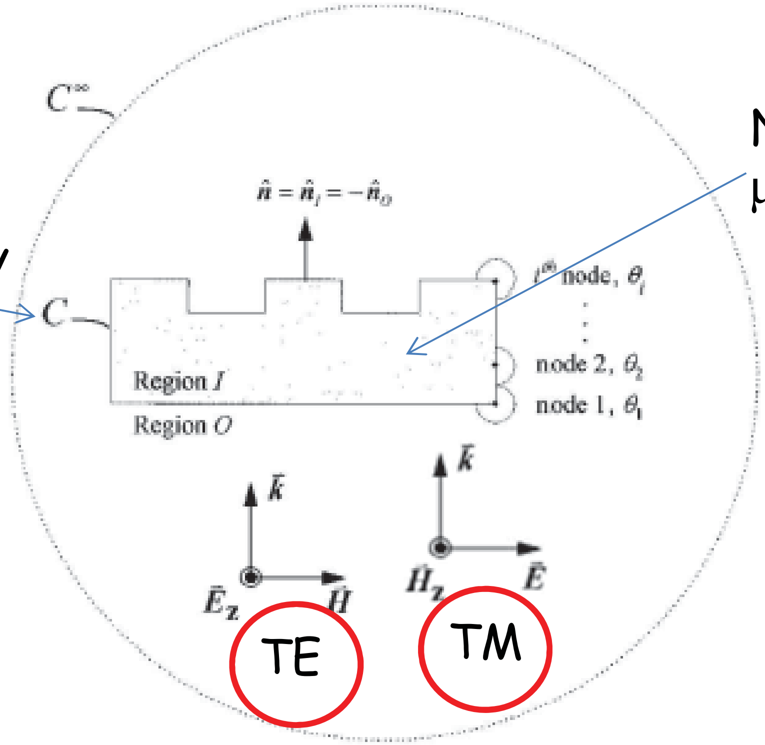


Incident radiation is represented by a source placed at infinity

Single Objects – Boundary Element Method

D. W. Prather et al., J. Opt. Soc. Am. A **14**, 34 (1997)

$$0 = \nabla^2 u_I^{tot}(\vec{r}) + k_I^2 u_I^{tot}(\vec{r}) \qquad \vec{r} \in I$$
$$-f(\vec{r}) = \nabla^2 u_O^{tot}(\vec{r}) + k_O^2 u_O^{tot}(\vec{r}) \qquad \vec{r} \in O$$

With $k_{I,O} = 2\pi\sqrt{\epsilon_{I,O}}/\lambda$ and the source term $f(\vec{r})$ at infinity

Integral solution to Maxwell Eq. (Kirchoff):

$$\begin{cases} u_I^{tot}(r) = \int_C \left(G_I(r,r')v_I^{tot}(r') - u_I^{tot}\frac{\partial G_I(r,r')}{\partial n_I} \right) dl' & r \in I \\ u_O^{tot}(r) = u_O^{inc}(r) + \left(\int_C + \int_{C\infty} \right) \left(u_O^{tot}(r')\frac{\partial G_O(r,r')}{\partial n_I} - G_O(r,r')v_O^{tot}(r') \right) dl' & r \in O \end{cases}$$

Where $v_{I,O}^{tot}(r) = \frac{\partial u_{I,O}^{tot}(r)}{\partial n_{I,O}}$ is the field component normal to contours

$u_O^{inc}(r) = \int_{C\infty} f(r')G_O(r,r')\, dl'$ is the incident field

Single Objects – Boundary Element Method

D. W. Prather et al., J. Opt. Soc. Am. A **14**, 34 (1997)

Boundary normal $\hat{n} = \hat{n}_I = -\hat{n}_O$

Green's function $G_{I,O}(r,r') = \frac{1}{4i} H_0^{(2)}(k_{I,O}|r-r'|)$

Continuity conditions
$$\begin{cases} u_I^{tot}(r) = u_O^{tot} \quad \text{per} \quad r \in C \\ \frac{1}{p_I}\frac{\partial u_I^{tot}(r)}{\partial n} = -\frac{1}{p_O}\frac{\partial u_O^{tot}(r)}{\partial n} \quad \text{per} \quad r \in C \end{cases}$$

Sommerfeld condition: scattered field decreasing to zero at infinity

$$\int_{C^\infty} \left(G_O(r,r') \frac{\partial u^{sc}(r')}{\partial n} - u^{sc}(r') \frac{\partial G_O(r,r')}{\partial n} \right) dl' = 0 \quad \text{per} \quad r \in O$$

With no object $u_O^{tot} = u_O^{inc}$

$$\int_{C} \left(G_O(r,r') \frac{\partial u^{inc}(r')}{\partial n} - u^{inc}(r') \frac{\partial G_O(r,r')}{\partial n} \right) dl' = 0 \quad \text{per} \quad r \in O$$

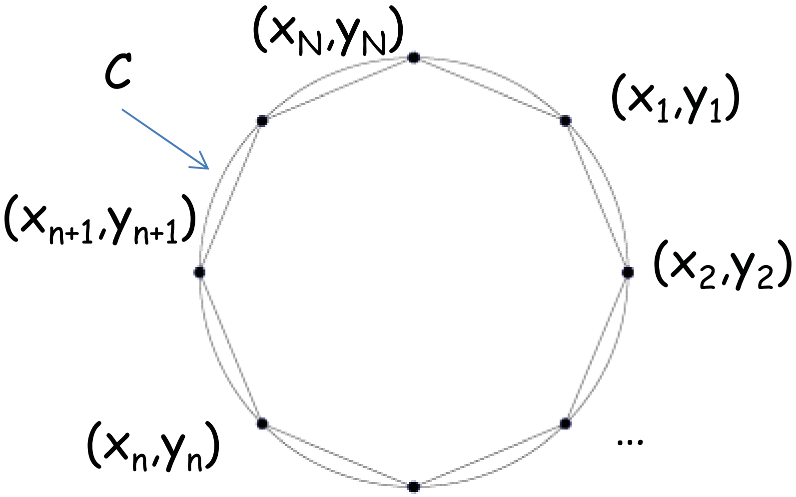
Single Objects – Boundary Element Method

D. W. Prather et al., J. Opt. Soc. Am. A **14**, 34 (1997)

Resulting equations:

$$\begin{cases} 0 = u^{sc}(r_s) + \int_C \left(u^{sc}(r') \frac{\partial G_I(r_s, r')}{\partial n} - p_I G_I(r_s, r') v^{sc}(r') \right) dl' \\ +u^{inc}(r_s) + \int_C \left(u^{inc}(r') \frac{\partial G_I(r_s, r')}{\partial n} - p_I G_I(r_s, r') v^{inc}(r') \right) dl' \qquad r_s \in I \\ 0 = u^{sc}(r_s) + \int_C \left(-u^{sc}(r') \frac{\partial G_O(r_s, r')}{\partial n} + p_O G_O(r_s, r') v^{sc}(r') \right) dl' \qquad r_s \in O \end{cases}$$

In numerical situations, integrals are discretized….



Using interpolating functions:

$$\phi_1(\xi) = \frac{1-\xi}{2}, \quad \phi_2(\xi) = \frac{1+\xi}{2}$$

Contour C is approximated by the follwing discrete set of points

$$r'(\xi) = r'(\hat{x}_n(\xi), \hat{y}_n(\xi))$$

$$\hat{x}_n(\xi) = x_n \phi_1(\xi) + x_{n+1} \phi_2(\xi)$$

$$\hat{y}_n(\xi) = y_n \phi_1(\xi) + y_{n+1} \phi_2(\xi)$$

Single Objects – Boundary Element Method

D. W. Prather et al., J. Opt. Soc. Am. A **14**, 34 (1997)

Following the same principle, scattered fields are discretized as well:

$$\mathbf{u}^{sc}(r_s(\xi)) = \sum_{n=1}^{N} (u_n^{sc}\phi_1(\xi) + u_{n+1}^{sc}\phi_2(\xi))$$

$$\mathbf{v}^{sc}(r_s(\xi)) = \sum_{n=1}^{N} (v_n^{sc}\phi_1(\xi) + v_{n+1}^{sc}\phi_2(\xi))$$

A set of 2N equations is obtained from the integral form:

$$\begin{bmatrix} ZI_{n,m} & -p_I YI_{n,m} \\ ZO_{n,m} & p_O YO_{n,m} \end{bmatrix} \begin{bmatrix} u_m^{sc} \\ v_m^{sc} \end{bmatrix} = \begin{bmatrix} -ZI_{n,m} & p_I YI_{n,m} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} u_m^{inc} \\ v_m^{inc} \end{bmatrix}$$

$$YI_{n,m} = \int_{-1}^{1} \left\{ \frac{\Delta l_n}{2}\phi_1(\xi) G_I(r'(\hat{x}_n, \hat{y}_n), r'_m) + \frac{\Delta l_{n-1}}{2}\phi_2(\xi) G_I(r'(\hat{x}_{n-1}, \hat{y}_{n-1}), r'_m) \right\} d\xi$$

$$ZO_{n,m} = \left(\frac{\theta_n}{2\pi}\right)\delta_{nm} - \int_{-1}^{1} \left\{ \frac{\Delta l_n}{2}\phi_1(\xi) \frac{\partial G_O(r'(\hat{x}_n, \hat{y}_n), r'_m)}{\partial n} + \frac{\Delta l_{n-1}}{2}\phi_2(\xi) \frac{\partial G_O(r'(\hat{x}_{n-1}, \hat{y}_{n-1}), r'_m)}{\partial n} \right\} d\xi$$

$$ZI_{n,m} = \left(1 - \frac{\theta_n}{2\pi}\right)\delta_{nm} + \int_{-1}^{1} \left\{ \frac{\Delta l_n}{2}\phi_1(\xi) \frac{\partial G_I(r'(\hat{x}_n, \hat{y}_n), r'_m)}{\partial n} + \frac{\Delta l_{n-1}}{2}\phi_2(\xi) \frac{\partial G_I(r'(\hat{x}_{n-1}, \hat{y}_{n-1}), r'_m)}{\partial n} \right\} d\xi$$

$$YO_{n,m} = \int_{-1}^{1} \left\{ \frac{\Delta l_n}{2}\phi_1(\xi) G_O(r'(\hat{x}_n, \hat{y}_n), r'_m) + \frac{\Delta l_{n-1}}{2}\phi_2(\xi) G_O(r'(\hat{x}_{n-1}, \hat{y}_{n-1}), r'_m) \right\} d\xi$$

Single Objects – Boundary Element Method

D. W. Prather et al., J. Opt. Soc. Am. A **14**, 34 (1997)

Once numerical values of fields on the discretized contour are known, the final scattered field can be computed according to

$$u^{sc}(r) = \int_C \left\{ u^{sc}(r') \frac{\partial G_O(r,r')}{\partial n} - p_O G_O(r,r') v^{sc}(r') \right\} dl' \qquad r \in O$$

$$0 = u^{sc}(r_s) + \int_C \left(u^{sc}(r') \frac{\partial G_I(r_s,r')}{\partial n} - p_I G_I(r_s,r') v^{sc}(r') \right) dl'$$

$$+u^{inc}(r_s) + \int_C \left(u^{inc}(r') \frac{\partial G_I(r_s,r')}{\partial n} - p_I G_I(r_s,r') v^{inc}(r') \right) dl' \qquad r_s \in I$$

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Complex Objects – Finite Element Method

Lot of literature on this topic!!

FEM Method

Integral method for solving Maxwell (Helmholtz) equations based on a discretization of object surface (in 2D) or volume (3D)

Exemplary commercial platform:
Comsol Multiphysics