

MODAL EXPANSION FOR THE 2D GREEN'S FUNCTION IN A NON-ORTHOGONAL COORDINATES SYSTEM

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Abstract—We present an efficient modal method to calculate the two-dimensional Green's function for electromagnetics in curvilinear coordinates. For this purpose the coordinate transformation based differential method, introduced for the numerical analysis of surface-relief gratings, is directly used with perfectly matched layers (PMLs). The covariant formalism Maxwell's equations, very convenient for the non-orthogonal coordinates formulation, also gives an unified analysis of PMLs. Numerical results for a line source placed above a perfectly conducting corrugated surface are presented.

1. INTRODUCTION

In 1994 Bérenger introduced the perfectly matched layers (PMLs) in finite-difference time-domain (FDTD) [1]. Since then the PMLs have been successfully combined with others methods in particular in the frequency domain. Chew and Weedon have shown in [2] the PML concept to be equivalent to a complex stretching on the coordinate space of Maxwell's equations. Then Teixeira *et al.* have interpreted this stretching as being equivalent to an analytical continuation of the coordinate space to a complex coordinate space [3]. More recently Teixeira et Chew proposed a unified analysis using differential forms [4]. In practice one main feature of the PMLs, which appears in many applications, lies in the fact that the PMLs allow to use modal expansion technics. For example consider a problem which is translation invariant in one direction. The computing domain is defined by placing in this direction two parallel perfectly electric conducting plates backed by a PML. So the original configuration is turned into a closed waveguide whereas the PMLs provide free space radiation conditions [5].

In optics the diffraction gratings have been widely studied since the fifties. The differential methods are based on the Floquet's expansion which is a generalized Fourier expansion. So it was very natural to apply the technics developed for studying gratings to non-periodic configurations by introducing PMLs [6]. Note that in this formalism the only pseudo-periodic condition must be verified whereas Dirichlet boundary conditions are imposed by the electric walls in the waveguide approach. In addition non-orthogonal co-ordinate systems can be successfully used in some gratings problems and then the covariant form of Maxwell's equations is really suitable [7].

The aim of this paper consists in computing the 2D Green's function in the so-called translation coordinates by using PMLs. Our purpose is to present a method which is very easy to implement. In the first section we introduce the tensorial covariant Maxwell's equations in which a change of metric is recognized as being equivalent to a change of medium. This interpretation is used in the second section to introduce PMLs in non-orthogonal coordinates. The third section is devoted to the 2D Green's function computation which is reduced to a numerical eigenvalue problem.

2. COVARIANT EM, METRIC, AND PML

The vector space \mathbb{R}^3 is identified to an affine space. At a point \mathbf{x} defined by its coordinates (x^1, x^2, x^3) in a basis $(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, the time-harmonic Maxwell's equations with electrical sources are represented in the covariant formulation

$$\xi^{ijk} \partial_j H_k = i\omega D^i + J^i, \quad \xi^{ijk} \partial_j E_k = -i\omega B^i \quad i, j, k = 1, 2, 3, \quad (1)$$

where $\partial_i = \frac{\partial}{\partial x^i}$ and ξ^{ijk} denotes the Levi-Civita tensor. These equations are written with the time convention $e^{i\omega t}$ and the Einstein's convention which are used throughout this paper. We emphasize that the covariant equations do not depend on a metric contrary to the constitutive relations. For example the contravariant components B^i and D^i are linked to the covariant components H_i and E_i in an homogeneous isotropic medium by

$$D^i = \varepsilon \sqrt{g} g^{ij} E_j, \quad B^i = \mu \sqrt{g} g^{ij} H_j, \quad (2)$$

where g^{ij} denote the contravariant components of metric tensor which are obtained by inverting the matrix constituted by the covariant components $g_{ij}(x^1, x^2, x^3)$. It is very important to remark that the relations Eq. (2) are also verified with the metric $g_{ij}(x^1, x^2, x^3) = \delta_{ij}$

and a medium whose magnetic and electric properties are characterized by the tensors

$$\varepsilon^{ij}(x^1, x^2, x^3) = \varepsilon \Lambda^{ij}(x^1, x^2, x^3), \quad \mu^{ij}(x^1, x^2, x^3) = \mu \Lambda^{ij}(x^1, x^2, x^3), \quad (3)$$

where

$$\Lambda^{ij}(x^1, x^2, x^3) = \sqrt{g} g^{ij}(x^1, x^2, x^3). \quad (4)$$

This medium exhibits the same behavior for the electric and the magnetic fields since the only tensor Λ is sufficient for expressing the constitutive relations. So the electromagnetic field expressed with a metric \mathbf{g} ($g_{ij} \neq \delta_{ij}$) in an homogeneous medium is the same as an electromagnetic field expressed with a Cartesian metric ($g_{ij} = \delta_{ij}$) in a medium defined by the original metric \mathbf{g} . More generally a change of the metric can be considered as a change of medium. For example let us consider a coordinate system (x^1, x^2, x^3) deduced from Cartesian coordinates $(x^1, x^2, x^3) = (x, y, z)$:

$$\Phi : (x^1, x^2, x^3) = (x, y, z) \quad \rightarrow \quad (x^1, x^2, x^3), \quad (5)$$

with

$$x^1(x) = \int_0^x s_1(x') dx', \quad x^2(y) = \int_0^y s_2(y') dy', \quad x^3(z) = \int_0^z s_3(z') dz'. \quad (6)$$

The change of coordinates induces the metric

$$g_{i'j'}(x^1, x^2, x^3) = \frac{\partial x^i}{\partial x^{i'}} \frac{\partial x^j}{\partial x^{j'}} \delta_{ij}. \quad (7)$$

Following the previous point of view we may associate the change of metric and the material tensor deduced from Eq. (4) and Eq. (7):

$$\Lambda(x^1, x^2, x^3) = \Lambda(x, y, z) = \begin{bmatrix} \frac{s_1(x)}{s_2(y)s_3(z)} & & \\ & \frac{s_2(y)}{s_1(x)s_3(z)} & \\ & & \frac{s_3(z)}{s_1(x)s_2(y)} \end{bmatrix}. \quad (8)$$

This tensor is the one which appears in the formalism proposed by Sacks *et al.* [8]. The physical realizability of material characterized

by Λ can be discussed but this is not necessary providing that the computed fields inside the material are regarded as nonphysical. The perfectly matched layer corresponds to complex valued functions s_i . This case may be mathematically interpreted as the analytic continuation of the metric to a complex metric.

Now assume the metric induced by the coordinate system (x^1, x^2, x^3) to be given by $g'_{ij}(x^1, x^2, x^3) = \delta_{ij}$. Then the natural vector basis (\mathbf{e}_i) of the system (x^1, x^2, x^3) become:

$$\mathbf{e}_i = \frac{\partial x^{i'}}{\partial x^i} \mathbf{e}_{i'}, \quad (9)$$

with $\|\mathbf{e}_{i'}\| = 1$. The modified metric of the system (x^1, x^2, x^3) is defined as

$$g'_{ij}(x^1, x^2, x^3) = g'_{ij}(x, y, z) = \begin{bmatrix} s_1^2(x) & & \\ & s_2^2(y) & \\ & & s_3^2(z) \end{bmatrix}, \quad (10)$$

and

$$\sqrt{g'} g'^{ij}(x^1, x^2, x^3) = \begin{bmatrix} \frac{s_2(y)s_3(z)}{s_1(x)} & & \\ & \frac{s_1(x)s_3(z)}{s_2(y)} & \\ & & \frac{s_1(x)s_2(y)}{s_3(z)} \end{bmatrix}. \quad (11)$$

Reporting Eq. (2) and Eq. (11) in Eq. (1) the covariant Maxwell's equations may be written as

$$\begin{aligned} \xi^{ijk} \partial_j E_k &= -i\omega\mu \frac{s_{i+1}s_{i+2}}{s_i} H_i, \\ \xi^{ijk} \partial_j H_k &= i\omega\varepsilon \frac{s_{i+1}s_{i+2}}{s_i} E_i + J^i, \quad \text{modulus 2,} \end{aligned} \quad (12)$$

where $i, j, k = x, y, z$. The basis \mathbf{e}_i is no more normalized since $\|\mathbf{e}_i\|^2 = s_i^2$. The coordinate system is in fact the system (x, y, z) but the metric has been modified.

3. PMLS IN A NON-ORTHOGONAL CURVILINEAR COORDINATES SYSTEM

The previous scheme, introduced for a PML medium, can be briefly recalled as follows:

- (i) a coordinate system (x^1, x^2, x^3) is deduced from the Cartesian system $(x^1, x^2, x^3) = (x, y, z)$ by Φ (Eq. (6)):

$$\Phi : g_{ij}(x^i) = \delta_{ij} \quad \longrightarrow \quad g_{ij}(x^{i'}), \quad (13)$$

- (ii) we consider the metric of this system to be equal the original one *i.e.* $g'_{ij}(x^{i'}) = \delta_{ij}$,
 (iii) by applying the inverse coordinate change we are led to a modified metric for the system (x^1, x^2, x^3)

$$\Phi^{-1} : g'_{ij}(x^{i'}) = \delta_{ij} \quad \longrightarrow \quad g'_{ij}(x^i). \quad (14)$$

The generalization of this scheme consists starting from any coordinates system (x^1, x^2, x^3) and proceeding with the same change Φ as previously:

$$\begin{aligned} \Phi : g_{ij}(x^i) &\rightarrow g_{ij}(x^{i'}), \\ \Phi^{-1} : g'_{ij}(x^{i'}) &= g_{ij}(x^{i'}) \rightarrow g'_{ij}(x^i). \end{aligned} \quad (15)$$

Practically the $g'_{ij}(x^{i'})$ can be directly deduced from the $g_{ij}(x^i)$ by considering these as functions of $x^{i'}$ instead of x^i , then replacing $\frac{\partial}{\partial x^i}$ by $\frac{\partial}{\partial x^{i'}}$ and finally computing the $g'_{ij}(x^i)$ by means of Φ^{-1} .

4. TRANSLATION COORDINATES

The so-called translation coordinate system [7] is defined from the Cartesian system by

$$\begin{aligned} x^1 &= x, \\ x^2 &= y - a(x) \\ x^3 &= z, \end{aligned} \quad (16)$$

where $a(x)$ is a periodic function with period d . Eq. (16) yields the natural metric

$$g_{ij}(x^1, x^2, x^3) = \begin{bmatrix} 1 + \frac{da}{dx^1} \frac{da}{dx^1} & \frac{da}{dx^1} & 0 & 0 \\ \frac{da}{dx^1} & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad (17)$$

The metric $g'_{ij}(x^1, x^2, x^3)$ is written by substituting $x^{1'}$ for x^1 :

$$g'_{ij}(x^1, x^2, x^3) = \begin{bmatrix} 1 + \frac{da}{dx^{1'}} \frac{da}{dx^{1'}} & \frac{da}{dx^{1'}} & 0 \\ \frac{da}{dx^{1'}} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (18)$$

The modified metric of the system (x^1, x^2, x^3) is obtained by means of the coordinates change Φ^{-1} :

$$g'_{ij}(x^1, x^2, x^3) = \frac{\partial x^k}{\partial x^i} \frac{\partial x^l}{\partial x^j} g'_{kl}(x^1, x^2, x^3). \quad (19)$$

Eq. (6), Eq. (18) and Eq. (19) yield

$$g'_{ij}(x^1, x^2, x^3) = \begin{bmatrix} s_1 s_1 \left(1 + \frac{da}{dx^{1'}} \frac{da}{dx^{1'}} \right) & s_1 s_2 \frac{da}{dx^{1'}} & 0 \\ s_1 s_2 \frac{da}{dx^{1'}} & s_2 s_2 & 0 \\ 0 & 0 & s_3 s_3 \end{bmatrix}, \quad (20)$$

where $\frac{da}{dx^{1'}}$ is considered as a function of x^1 .

5. 2D GREEN'S FUNCTION

For the purpose of this paper we assume s_2 and s_3 to be equal to one and we simplify the notation by substituting s for s_1 . From Eq. (20) we obtain

$$\sqrt{g'} g'^{ij}(x^1, x^2, x^3) = \begin{bmatrix} \frac{1}{s} & -\dot{a} & 0 \\ -\dot{a} & s(1 + \dot{a}\dot{a}) & 0 \\ 0 & 0 & s \end{bmatrix}. \quad (21)$$

where

$$\dot{a} = \frac{da}{dx^{1'}}(x^1)$$

We consider any problem which is invariant with the $z = x^3$ direction ($\partial_3 = 0$). In a domain without source ($J^i = 0$) Eqs. (1) and (2) yield the propagation equation written in the translation coordinate system

$$\left[\frac{1}{s} \partial_1 \frac{1}{s} \partial_1 - \left(\frac{1}{s} \partial_1 \dot{a} + \dot{a} \frac{1}{s} \partial_1 \right) \partial_2 + (1 + \dot{a}\dot{a}) \partial_2^2 + \omega^2 \epsilon \mu \right] \Psi(x^1, x^2) = 0 \quad (22)$$

where Ψ holds for E_z or H_z . This equation can be obtained by substituting the operator $\frac{1}{s}\frac{\partial}{\partial_1}$ for $\frac{\partial}{\partial_1}$ in the equation obtained in the original translation coordinate system Eq. (16). The second order differential equation can be written as two first order coupled equations:

$$\begin{bmatrix} -i\frac{1}{s}\partial_1\dot{a} - i\dot{a}\frac{1}{s}\partial_1 & 1 + \dot{a}\dot{a} \\ 1 & 0 \end{bmatrix} i\partial_2 \begin{bmatrix} \Psi \\ \dot{\Psi} \end{bmatrix} = \begin{bmatrix} \frac{1}{s}\partial_1\frac{1}{s}\partial_1 + \omega^2\varepsilon\mu & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \Psi \\ \dot{\Psi} \end{bmatrix} \quad (23)$$

where $\dot{\Psi} = i\partial_2\Psi$. Since the functions \dot{a} and s depend on the only x^1 variable we may assume an exponential x^2 dependence $e^{-i\beta x^2}$ and replace the operator ∂_2 by the $-i\beta$ coefficient. Assuming \dot{a} to be a periodic function, the solutions may be approximated by expanding Ψ into Fourier basis $e_n(x^1) = \exp(-i\alpha_n x^1)$ where $\alpha_n = n2\pi x^1/d$, $n \in \mathbf{Z}$ and d is the period.

$$\Psi(x^1, x^2) = e^{-i\beta x^2} \sum_n \Psi_n(\beta) e_n(x^1). \quad (24)$$

In Fourier space Eq. (23) yields the matrix equation

$$\begin{bmatrix} -\mathbf{s}^{-1}\boldsymbol{\alpha}\mathbf{s}^{-1}\boldsymbol{\alpha} + \omega^2\varepsilon\mu\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \Psi \\ \dot{\Psi} \end{bmatrix} = \beta \begin{bmatrix} -\mathbf{s}^{-1}\boldsymbol{\alpha}\dot{\boldsymbol{a}} - \dot{\boldsymbol{a}}\mathbf{s}^{-1}\boldsymbol{\alpha} & \mathbf{I} + \dot{\boldsymbol{a}}\dot{\boldsymbol{a}} \\ \mathbf{I} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \Psi \\ \dot{\Psi} \end{bmatrix} \quad (25)$$

where the bold symbols denote matrices. $\boldsymbol{\alpha}$ is a diagonal matrix formed by α_n , \mathbf{s} and $\dot{\boldsymbol{a}}$ are Toeplitz matrices whose the mn element is the $(m - n)$ Fourier coefficient of the corresponding function and \mathbf{s}^{-1} is the inverse matrix. Ψ and $\dot{\Psi}$ are column vectors formed by the Fourier coefficients of Ψ and $\dot{\Psi}$ with respect to x^1 . So the Fourier expansion results in a fully discrete spectrum of eigen modes

$$\Psi_q(x^1, x^2) = e^{-i\beta_q x^2} \sum_n \Psi_{nq} e_n(x^1) \quad (26)$$

where β_q is an eigenvalue of Eq. (25) and Ψ_{nq} the Fourier coefficient of the corresponding eigen function Ψ_q . In this way we can obtain a modal expansion very suitable to calculate the radiated field of a periodic electric source with the only condition that the period of the source is the same as the period d of the function $\dot{a}(x^1)$. Numerically the infinite matrices in Eq. (25) are necessary truncated. The eigenvalues

can be divided into two sets. The first set, Σ^- , contains the negative real eigenvalues and the complex eigenvalues having positive imaginary parts. The second set, Σ^+ , contains those with the opposite signs.

The 2D Green's function $G(x^1, x^2)$, periodic with respect to x^1 , obeys the equation:

$$\begin{aligned} & \left[\frac{1}{s} \partial_1 \frac{1}{s} \partial_1 - \left(\frac{1}{s} \partial_1 \dot{a} + \dot{a} \frac{1}{s} \partial_1 \right) \partial_2 + (1 + \dot{a}\dot{a}) \partial_2^2 + \omega^2 \epsilon \mu \right] G(x^1, x^2) \\ &= \delta(x^2 - X^2) \sum_n \delta(x^1 - X^1 - nd) \end{aligned} \quad (27)$$

Since

$$\sum_n \delta(x^1 - X^1 - nd) = \sum_n \frac{1}{d} e_n^*(X^1) e_n(x^1), \quad (28)$$

where the asterisk refers to the complex conjugate, the Green's function may be expanded in Fourier series

$$G(x^1, x^2) = \sum_n G_n(x^2) e_n(x^1), \quad (29)$$

and Eq. (27) can be converted into a matrix equation in Fourier space:

$$\begin{aligned} \mathbf{L}[G_n(x^2)] + \mathbf{M}[\partial_2 G_n(x^2)] + \mathbf{N}[\partial_2^2 G_n(x^2)] + \omega^2 \epsilon \mu [G_n(x^2)] \\ = \delta(x^2 - X^2) \frac{1}{d} [e_n^*(X^1)], \end{aligned} \quad (30)$$

with

$$\begin{aligned} \mathbf{L} &= -\mathbf{s}^{-1} \boldsymbol{\alpha} \mathbf{s}^{-1} \boldsymbol{\alpha}, \\ \mathbf{M} &= i \mathbf{s}^{-1} \boldsymbol{\alpha} \dot{\mathbf{a}} + i \dot{\mathbf{a}} \mathbf{s}^{-1} \boldsymbol{\alpha}, \\ \mathbf{N} &= \mathbf{I} + \dot{\mathbf{a}} \dot{\mathbf{a}}. \end{aligned}$$

From Eq. (26) the functions $G_n(x^2)$ may be written as a modal expansion:

$$G_n(x^2) = \sum_q A_q \Psi_{nq} e^{-i\beta_q x^2}. \quad (31)$$

In free space the radiation conditions in the x^2 direction are enforced by holding the set of eigenvalues Σ^+ in the domain $x^2 > X^2$ and the

set Σ^- in the domain $x^2 < X^2$ Considering the derivative ∂_2 within the sense of distributions Eq. (30) yields the system of equations

$$\begin{aligned} \mathbf{M}[G_n^+(X^2) - G_n^-(X^2)] + \mathbf{N}[\partial_2 G_n^+(X^2) - \partial_2 G_n^-(X^2)] &= \frac{1}{d}[e_n^*(X^1)], \\ \mathbf{N}[G_n^+(X^2) - G_n^-(X^2)] &= 0, \end{aligned} \quad (32)$$

and

$$\begin{aligned} \mathbf{N}[\partial_2 G_n^+(X^2) - \partial_2 G_n^-(X^2)] &= \frac{1}{d}[e_n^*(X^1)], \\ [G_n^+(X^2) - G_n^-(X^2)] &= 0, \end{aligned} \quad (33)$$

which provides the numerical values of the coefficients A_q .

6. RESULTS

In this section, we provide numerical examples to illustrate the effectiveness of our formulation. The first one deals with the radiation of an electric current line source in free space. In that case it can be shown that the exact solution for the electric field is given by:

$$E_z(x, y) = H_0^2 \left(k \left((x - X^1)^2 + (y - X^2)^2 \right)^{1/2} \right) \quad (34)$$

where H_0^2 is the zeroth order Hankel function of the second kind and k the wave number. Fig. 1 illustrates the geometry of our numerical experiment. In Eq. (16), we have used the function $a(x) = .5 * h(1 + \cos \frac{2\pi x}{d})$ with $h = \lambda$, $d = 10\lambda$. The source is located at $(X^1, X^2) = (d/2, -\lambda/10)$. The PML function has been chosen to be

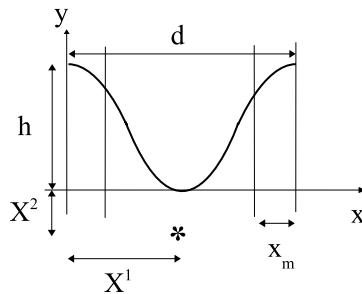


Figure 1. A line source below a sinusoidal coordinate line.

the most simple one :

$$s(x^1) = \begin{cases} 1 - i\eta & \text{if } 0 < x^1 < x_m \\ 1 & \text{if } x_m < x^1 < d - x_m \\ 1 - i\eta & \text{if } d - x_m < x^1 < d \end{cases} \quad (35)$$

with $\eta = 1,5$ and $x_m = \lambda/10$. Fig. 2 shows a comparison of the imaginary part of the electric field at $x^2 = 0$ obtained from the closed form solution and from the modal solution. It is seen that agreement is excellent even close to the source. The second example is for a line source located at the focus of a parabola. The width of the parabola is $d = 15\lambda$, and the focus is $f = d/4$. (see Fig. 3). Fig. 4 represents a map of the total electric field.

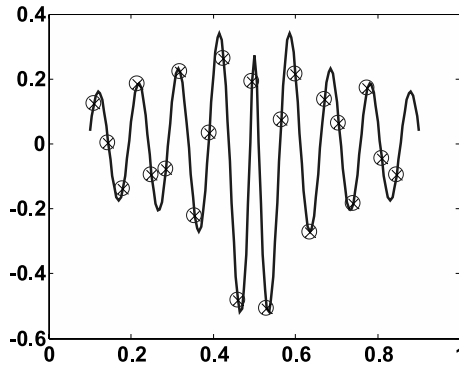


Figure 2. Radiation of a line source on a sinusoidal line. The curve represents the imaginary part of the zeroth order Hankel function of the second kind as a function of x^1 calculated at $x^2 = y - a(x)$. The full line is for the closed-form solution and crosses inside circles are for the modal solution. The geometry is that of Fig. 1 with $X^1 = .5d$, $X^2 = .1\lambda$, $d = 10\lambda$, $\lambda = 1$.

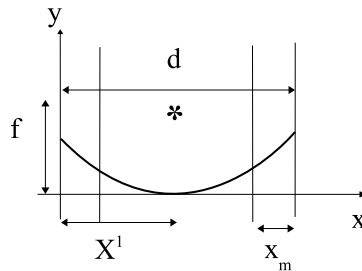


Figure 3. A line source at the focus of perfectly conducting parabola.

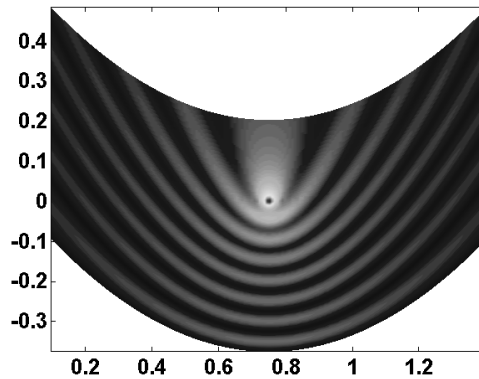


Figure 4. Modulus of the electric field radiated by a line source at the focus of a parabola. The geometry is that of Fig. 3. The parameters are: $\lambda = .1$, $d = 15\lambda$, $f = \frac{d}{4}$.

7. CONCLUSION

In this paper we have introduced complex coordinate stretching in the so-called translation coordinate system. We have computed the 2D free-space Green function using a numerical modal technic in conjunction with Fourier expansions. Hence, as expected, we have verified that complex coordinate stretching behaves as a radiation condition in a general non orthogonal coordinate system. However, in our opinion, the most interesting part of this preliminary work is the fact that we have obtained a series expansion linked to any coordinate system. Thus, when solving a given problem where radiation occurs, we may choose the most convenient coordinate system. Moreover the above approach can be extended to non homogeneous media in a straightforward manner.

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