Vector Based 3D FEM for Electromagnetic Scattering

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1 Introduction

We have formulated a vector based Finite Element Method (FEM) to numerically simulate Electromagnetic Scattering from a 3D dielectric object. We primarily referred to *The Finite Element Method in Electromagnetics* [1] by Jianming Jin among other resources. Matrix assembly and subsequent steps to evaluate the far-field have been implemented in C++. We are currently verifying the model for Mie scattering from a homogeneous dielectric sphere.

2 Helmholtz Equation

In a space free of stationary charge sources (but possibly having known current sources $\vec{J}(r)$), the spatial Maxwell's equations are given by

$$\nabla \times \vec{E} = -j\omega\mu_0\vec{H} \tag{1}$$

$$\nabla \times \vec{H} = j\omega\epsilon\vec{E} + \vec{J} \tag{2}$$

This gives rise to the Helmholtz equation

$$\vec{R}_E = \nabla \times (\nabla \times \vec{E}) - k_0^2\epsilon_r\vec{E} + j\omega\mu_0\vec{J} = 0 \tag{3}$$

where ϵ_r is a function of space, and $k_0^2 = \omega^2\mu_0\epsilon_0$. We consider a non-magnetic material ($\mu_r = 1$) in the analysis.

3 Weighted Residual formulation

Let the testing function be denoted by $\vec{T}(\vec{r})$. Weighted residual method sets $\vec{R}$ to zero in a weighted manner as follows -

$$\int_\Omega \vec{T} \cdot \vec{R}\, dV = \int_\Omega \vec{T} \cdot \Big(\nabla \times (\nabla \times \vec{E}) - k_0^2\epsilon_r\vec{E} + j\omega\mu_0\vec{J}\Big)\, dV = 0 \tag{4}$$

This is a volume integral over the entire computational domain Ω, and $dV = dx\, dy\, dz$. From vector calculus, we know $\vec{A} \cdot (\nabla \times \vec{B}) = \vec{B} \cdot (\nabla \times \vec{A}) - \nabla \cdot (\vec{A} \times \vec{B})$. Choosing $\vec{A} = \vec{T}$ and $\vec{B} = (\nabla \times \vec{E})$,

$$\vec{T} \cdot \Big(\nabla \times (\nabla \times \vec{E})\Big) = (\nabla \times \vec{E}) \cdot (\nabla \times \vec{T}) - \nabla \cdot (\vec{T} \times (\nabla \times \vec{E})) \tag{5}$$

The integral in Equation (4) can hence be expanded as

$$\boxed{\int_\Omega \Big[(\nabla \times \vec{T}) \cdot (\nabla \times \vec{E}) - k_0^2\epsilon_r\vec{T} \cdot \vec{E} + j\omega\mu_0\vec{T} \cdot \vec{J}\Big]\, dV = -\oint_\Gamma \vec{T} \cdot \Big(\hat{n} \times (\nabla \times \vec{E})\Big)\, dS} \tag{6}$$

To get the RHS, we have used the 3D Divergence theorem $\int_\Omega \nabla \cdot \vec{F}\, dV = \oint_\Gamma \vec{F} \cdot \hat{n}\, dS$. Γ is the closed surface enclosing our 3D computational domain Ω, and $\hat{n}$ is the outward unit normal evaluated on Γ.
In our case, $\vec{F} = \left(\vec{T} \times (\nabla \times \vec{E})\right)$. Hence

$$\int_\Omega \nabla \cdot \left(\vec{T} \times (\nabla \times \vec{E})\right) dV = \oint_\Gamma \left(\vec{T} \times (\nabla \times \vec{E})\right) \cdot \hat{n} dS \tag{7}$$

$$= -\oint_\Gamma \vec{T} \cdot \left(\hat{n} \times (\nabla \times \vec{E})\right) dS \tag{8}$$

3.1 Incident Field problem ($\vec{J} = 0$)

For the case when $\vec{J} = 0$, we use the 1st order Radiation Boundary Condition (RBC) at Γ as

$$\hat{n} \times (\nabla \times \vec{E}_s) = -jk_0\sqrt{\epsilon_r}\left(\hat{n} \times (\hat{n} \times \vec{E}_s)\right) \tag{9}$$

where $\vec{E}_s = \vec{E} - \vec{E}_{inc}$ is the scattered field.

$$\hat{n} \times (\nabla \times (\vec{E} - \vec{E}_{inc})) = -jk_0\sqrt{\epsilon_r}\left(\hat{n} \times (\hat{n} \times (\vec{E} - \vec{E}_{inc}))\right) \tag{10}$$

$$\implies \quad \hat{n} \times (\nabla \times \vec{E}) = \hat{n} \times \left[\nabla \times \vec{E}_{inc} + jk_0\sqrt{\epsilon_r}(\hat{n} \times \vec{E}_{inc}) - jk_0\sqrt{\epsilon_r}(\hat{n} \times \vec{E})\right] \tag{11}$$

Using the above result in Equation (8), we have

$$-\oint_\Gamma \vec{T} \cdot (\hat{n} \times (\nabla \times \vec{E}))\, dS = -\oint_\Gamma \vec{T} \cdot (\hat{n} \times (\nabla \times \vec{E}_{inc}))\, dS - jk_0 \oint_\Gamma \sqrt{\epsilon_r}\vec{T} \cdot (\hat{n} \times (\hat{n} \times \vec{E}_{inc}))\, dS + jk_0 \oint_\Gamma \sqrt{\epsilon_r}\vec{T} \cdot (\hat{n} \times (\hat{n} \times \vec{E}))\, dS \tag{12}$$

Using the above result in the RHS of Equation (6), we finally have

$$\boxed{\begin{aligned}\int_\Omega \left[(\nabla \times \vec{T}) \cdot (\nabla \times \vec{E}) - k_0^2\epsilon_r\vec{T} \cdot \vec{E}\right] dV - jk_0 \oint_\Gamma \sqrt{\epsilon_r}\vec{T} \cdot (\hat{n} \times (\hat{n} \times \vec{E}))\, dS \\ = \oint_\Gamma \left[-jk_0\sqrt{\epsilon_r}\left(\vec{T} \cdot (\hat{n} \times (\hat{n} \times \vec{E}_{inc})\right) - \vec{T} \cdot \left(\hat{n} \times (\nabla \times \vec{E}_{inc})\right)\right] dS\end{aligned}} \tag{13}$$

This is the FEM Weak Form for $\vec{J} = 0$ in the Total Field (TF) formalism.

- The RHS is a surface integral in terms of the incident field $\vec{E}_{inc}$ (known) evaluated on Γ.
- The LHS has a volume integral and a surface integral: the volume integral is in terms of the total field $\vec{E}$ (unknown) and ϵ_r (known) evaluated everywhere in Ω, while the surface integral is in terms of the total field $\vec{E}$ evaluated on Γ.

3.2 Antenna Radiation problem ($\vec{J} \neq 0$)

In this case, we have radiating current sources $\vec{J}$ inside Ω, but no separate Incident Field. Hence RBC is directly applied on the Total Field as

$$\hat{n} \times (\nabla \times \vec{E}) = -jk_0\sqrt{\epsilon_r}\left(\hat{n} \times (\hat{n} \times \vec{E})\right) \tag{14}$$

In this case, the weak form after applying (14) to the RHS term (8) becomes

$$\boxed{\int_\Omega \left[(\nabla \times \vec{T}) \cdot (\nabla \times \vec{E}) - k_0^2 \epsilon_r \vec{T} \cdot \vec{E}\right] dV - jk_0 \oint_\Gamma \sqrt{\epsilon_r} \left[\vec{T} \cdot (\hat{n} \times (\hat{n} \times \vec{E})\right] dS = -j\omega\mu_0 \int_\Omega \vec{T} \cdot \vec{J}\, dV} \tag{15}$$

4 Galerkin Testing

We construct the scalar function $\Phi(\vec{T}, \vec{E})$ as

$$\Phi(\vec{T}, \vec{E}) := \int_\Omega \left[(\nabla \times \vec{T}) \cdot (\nabla \times \vec{E}) - k_0^2 \epsilon_r \vec{T} \cdot \vec{E}\right] dV - jk_0 \oint_\Gamma \sqrt{\epsilon_r} \vec{T} \cdot (\hat{n} \times (\hat{n} \times \vec{E}))\, dS \tag{16}$$

Evidently $\Phi(\vec{T}, \vec{E})$ is linear in $\vec{E}$, that is

$$\Phi(\vec{T}, c_1\vec{E_1} + c_2\vec{E_2}) = c_1\Phi(\vec{T}, \vec{E_1}) + c_2\Phi(\vec{T}, \vec{E_2}) \tag{17}$$

Likewise we define the scalar function $b(\vec{T})$ as

$$\boxed{b(\vec{T}) := \begin{cases} \oint_\Gamma \left[-jk_0\sqrt{\epsilon_r}\left(\vec{T} \cdot (\hat{n} \times (\hat{n} \times \vec{E}_{inc})\right) - \vec{T} \cdot \left(\hat{n} \times (\nabla \times \vec{E}_{inc})\right)\right] dS, & \vec{J} = 0 \\ -j\omega\mu_0 \int_\Omega \vec{T} \cdot \vec{J}\, dV, & \vec{J} \neq 0 \end{cases}} \tag{18}$$

The FEM weak form then simply reads $\Phi(\vec{T}, \vec{E}) = b(\vec{T})$

Now suppose there are a <u>total of N edges in Ω after meshing</u>. Corresponding to each global edge j is a global basis function $\vec{T_j}$. We expand the total field $\vec{E}$ in Ω in terms of the global basis functions as

$$\vec{E} = \sum_{j=1}^{N} u_j \vec{T_j} \tag{19}$$

There are N unknown coefficients we have to solve for. Galerkin's method achieves this by testing the weak form with each of the N global basis functions $\vec{T_i}$. For $i = 1 \ldots N$, we have N equations of the form

$$\sum_{j=1}^{N} u_j \Phi(\vec{T_i}, \vec{T_j}) = b(\vec{T_i}) \tag{20}$$

This can hence be expressed compactly as the matrix equation

$$\mathbf{Au} = \mathbf{b} \tag{21}$$

where

$$\boxed{\mathbf{A}_{ij} = \Phi(\vec{T_i}, \vec{T_j}) = \int_\Omega \left[(\nabla \times \vec{T_i}) \cdot (\nabla \times \vec{T_j}) - k_0^2 \epsilon_r \vec{T_i} \cdot \vec{T_j}\right] dV - jk_0 \oint_\Gamma \sqrt{\epsilon_r}\, \vec{T_i} \cdot (\hat{n} \times (\hat{n} \times \vec{T_j}))\, dS} \tag{22}$$

and

$$\boxed{\mathbf{b}_i = b(\vec{T_i})} \tag{23}$$

Solving the Matrix Equation (21) efficiently will give us the coefficients $\mathbf{u}$. Then by Equation (19), we obtain the approximate total field $\vec{E}$ everywhere in the computational domain Ω.

5 Scalar basis functions for the Tetrahedral Element[1]

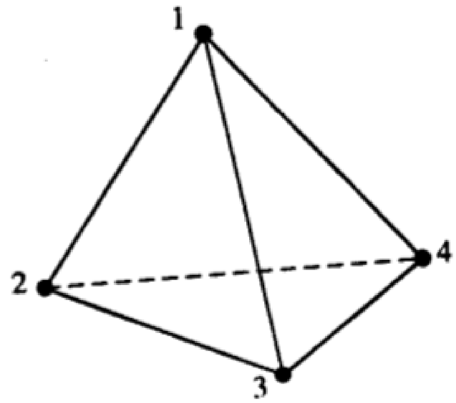

Figure 1: Tetrahedral element

The volume of the element V_e is given by

$$V_e = \frac{1}{6}\begin{vmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x_4 \\ y_1 & y_2 & y_3 & y_4 \\ z_1 & z_2 & z_3 & z_4 \end{vmatrix} \tag{24}$$

We define 4 scalar basis functions $L_j(x, y, z)$ $j = 1, 2, 3, 4$ corresponding to the four nodes.

$$L_1(x,y,z) = \frac{V_1}{V_e} = \frac{1}{6V_e}\begin{vmatrix} 1 & 1 & 1 & 1 \\ x & x_2 & x_3 & x_4 \\ y & y_2 & y_3 & y_4 \\ z & z_2 & z_3 & z_4 \end{vmatrix} \qquad L_2(x,y,z) = \frac{V_2}{V_e} = \frac{1}{6V_e}\begin{vmatrix} 1 & 1 & 1 & 1 \\ x_1 & x & x_3 & x_4 \\ y_1 & y & y_3 & y_4 \\ z_1 & z & z_3 & z_4 \end{vmatrix}$$

$$L_3(x,y,z) = \frac{V_3}{V_e} = \frac{1}{6V_e}\begin{vmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x & x_4 \\ y_1 & y_2 & y & y_4 \\ z_1 & z_2 & z & z_4 \end{vmatrix} \qquad L_4(x,y,z) = \frac{V_4}{V_e} = \frac{1}{6V_e}\begin{vmatrix} 1 & 1 & 1 & 1 \\ x_1 & x_2 & x_3 & x \\ y_1 & y_2 & y_3 & y \\ z_1 & z_2 & z_3 & z \end{vmatrix}$$

- The definition is valid when (x, y, z) is inside the element. Outside element e, all L_j^e are zero.
- All are linear functions of x, y, z.
- L_j takes value 1 at (x_j, y_j, z_j) and 0 everywhere on the opposite face.

6 Evaluating the scalar basis functions

The volume of each element in terms of the node coordinates is given by (simplified in MATLAB)

$$\begin{aligned} V_e = \ & \frac{1}{6}(x_1y_3z_2 - x_1y_2z_3 + x_2y_1z_3 - x_2y_3z_1 - x_3y_1z_2 + x_3y_2z_1 \\ & +x_1y_2z_4 - x_1y_4z_2 - x_2y_1z_4 + x_2y_4z_1 + x_4y_1z_2 - x_4y_2z_1 \\ & -x_1y_3z_4 + x_1y_4z_3 + x_3y_1z_4 - x_3y_4z_1 - x_4y_1z_3 + x_4y_3z_1 \\ & +x_2y_3z_4 - x_2y_4z_3 - x_3y_2z_4 + x_3y_4z_2 + x_4y_2z_3 - x_4y_3z_2) \end{aligned}$$

$$L_1(x,y,z) = \frac{1}{6V_e}(a_1 + b_1 x + c_1 y + d_1 z) \qquad L_2(x,y,z) = \frac{1}{6V_e}(a_2 + b_2 x + c_2 y + d_2 z) \tag{25}$$

$$L_3(x,y,z) = \frac{1}{6V_e}(a_3 + b_3 x + c_3 y + d_3 z) \qquad L_4(x,y,z) = \frac{1}{6V_e}(a_4 + b_4 x + c_4 y + d_4 z) \tag{26}$$

Coefficients of L_1 are given by

$$a_1 = \begin{vmatrix} x_2 & x_3 & x_4 \\ y_2 & y_3 & y_4 \\ z_2 & z_3 & z_4 \end{vmatrix} \qquad b_1 = -\begin{vmatrix} 1 & 1 & 1 \\ y_2 & y_3 & y_4 \\ z_2 & z_3 & z_4 \end{vmatrix} \qquad c_1 = \begin{vmatrix} 1 & 1 & 1 \\ x_2 & x_3 & x_4 \\ z_2 & z_3 & z_4 \end{vmatrix} \qquad d_1 = -\begin{vmatrix} 1 & 1 & 1 \\ x_2 & x_3 & x_4 \\ y_2 & y_3 & y_4 \end{vmatrix} \tag{27}$$

Trick to find coeffs a_i, b_i, c_i, d_i for i=2,3,4 :
Replace x_i, y_i, z_i with x_1, y_1, z_1, and add an overall minus sign (in the above determinants)

7 Local Vector basis functions for the Tetrahedral Element

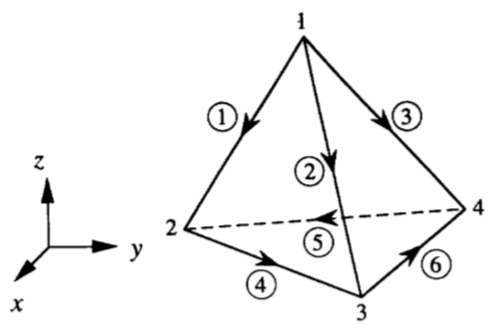

Figure 2: Tetrahedral element, with locally numbered nodes and directed edges. The direction of edge number 5 is wrong above.

We can now construct 6 local vector basis functions for the tetrahedral element. These correspond to the 6 directed edges, as seen in Fig. 2.

Corresponding to edge-1 (connecting node-1 and node-2), we define the vector basis function $\vec{T}_1^e$ as

$$\vec{T}_1^e = l_1 \left(L_1 \nabla L_2 - L_2 \nabla L_1 \right) \tag{28}$$

(l_1 is the length of edge-1)

It has three important properties:

- $\nabla \cdot \vec{T}_1^e = 0$
- $\nabla \times \vec{T}_1^e = 2 l_1 (\nabla L_1 \times \nabla L_2)$
- $\hat{e}_1 \cdot \vec{T}_1^e = 1$ where $\hat{e}_1$ is the unit vector of edge 1 (directed from node 1 to node 2)

The last point can be understood easily. Since L_1 is linear, its gradient is a constant vector. Further, since it varies from one at node-1 to zero at node-2, $\hat{e}_1 \cdot \nabla L_1 = -1/l_1$. Similarly $\hat{e}_1 \cdot \nabla L_2 = 1/l_1$. Therefore

$$\hat{e}_1 \cdot \vec{T}_1^e = (L_1 + L_2)|_{on\ edge\ 1} = 1 \tag{29}$$

To generalize, the vector basis function $\vec{T}_i^e$ corresponding to edge i of element e is given by

$$\boxed{\vec{T}_i^e = l_i(L_{i_1}\nabla L_{i_2} - L_{i_2}\nabla L_{i_1})} \tag{30}$$

where i_1 and i_2 are the (local) nodes joining which gives (local) edge i (in element e).

Edge i	Node i_1	Node i_2
1	1	2
2	1	3
3	1	4
4	2	3
5	4	2
6	3	4

Table 1: Local numbering of edges and nodes. Edge 5 is wrong above.

8 Global basis functions & Evaluating the Matrix elements

To recall, the computational domain Ω has a total of N edges. We have the global matrix equation $\mathbf{Au} = \mathbf{b}$, and $\mathbf{A}$ is the $N \times N$ FEM matrix whose elements we have to determine.

$$A_{ij}^{N\times N} = \Phi(\vec{T}_i, \vec{T}_j) = \int_\Omega \left[(\nabla \times \vec{T}_i) \cdot (\nabla \times \vec{T}_j) - k_0^2 \epsilon_r \vec{T}_i \cdot \vec{T}_j \right] dV - jk_0 \oint_\Gamma \sqrt{\epsilon_r}\, \vec{T}_i \cdot (\hat{n} \times (\hat{n} \times \vec{T}_j))\, dS \quad (31)$$

Note that $\vec{T}_i$ and $\vec{T}_j$ here are global basis functions corresponding to global edges i and j respectively.

The global basis function $\vec{T}_i$ is the sum of local basis functions $\vec{T}_k^e$ which have a constant component along the global edge i.

$$\vec{T}_i = \sum_{\substack{e \\ e\cap i \neq \phi}} \vec{T}_k^e \quad (32)$$

$i \longrightarrow k$ is the global to local mapping of edges. This means that global edge i is the same as local edge k in **all** elements e it belongs to. In our problem, $i \in \{1 \dots N\}$ while $k \in \{1 \dots 6\}$ (clearly a many-one map)

Now lets the break the term A_{ij} as

$$\boxed{A_{ij} = P_{ij} - Q_{ij} + R_{ij} - S_{ij}} \quad (33)$$

where

$$P_{ij} = \int_\Omega (\nabla \times \vec{T}_i) \cdot (\nabla \times \vec{T}_j)\ dV \quad (34)$$

$$Q_{ij} = k_0^2 \int_\Omega \epsilon_r\, \vec{T}_i \cdot \vec{T}_j\ dV \quad (35)$$

$$R_{ij} = jk_0 \oint_\Gamma \sqrt{\epsilon_r} \vec{T}_i \cdot \vec{T}_j\ dS \qquad S_{ij} = jk_0 \oint_\Gamma \sqrt{\epsilon_r} (\vec{T}_i \cdot \hat{n})(\vec{T}_j \cdot \hat{n})\ dS \quad (36)$$

In what follows, we will use the global to local edge mapping $i \longrightarrow k$ and $j \longrightarrow m$.

Mental Picture: Geometrically, each global basis function is non-zero in a pentagonal/hexagonal bipyramid whose central axis is the global edge. Two distinct bipyramids typically intersect at 0 or 1 or 2 tetrahedral elements.

8.1 P

From the previous section, we know that

$$\nabla \times \vec{T}_k^e = 2 l_k^e (\nabla L_{k_1}^e \times \nabla L_{k_2}^e) \quad (37)$$

Since $L = \frac{1}{6V}(a + bx + cy + dz)$, $\nabla L = \frac{1}{6V}(b, c, d)$.

$$\nabla L_{k_1}^e \times \nabla L_{k_2}^e = \frac{1}{36 V_e^2} \Big((c_{k_1} d_{k_2} - c_{k_2} d_{k_1}), (d_{k_1} b_{k_2} - d_{k_2} b_{k_1}), (b_{k_1} c_{k_2} - b_{k_2} c_{k_1}) \Big)_e \quad (38)$$

$$P_{ij} = \int_\Omega (\nabla \times \vec{T}_i) \cdot (\nabla \times \vec{T}_j) dV \quad (39)$$

$$= \sum_e \int_\Omega (\nabla \times \vec{T}_k^e) \cdot (\nabla \times \vec{T}_m^e) dV \quad (40)$$

$$
\boxed{\begin{aligned}
P_{ij} = \frac{l_k^e l_m^e}{324} \sum_e \frac{1}{V_e^3} \Big[&(c_{k_1} d_{k_2} - c_{k_2} d_{k_1})(c_{m_1} d_{m_2} - c_{m_2} d_{m_1}) + (d_{k_1} b_{k_2} - d_{k_2} b_{k_1})(d_{m_1} b_{m_2} - d_{m_2} b_{m_1}) \qquad (41)\\
&+ (b_{k_1} c_{k_2} - b_{k_2} c_{k_1})(b_{m_1} c_{m_2} - b_{m_2} c_{m_1})\Big]_e \qquad (42)
\end{aligned}}
$$

Sum is over elements e which have both i $(k_1 - k_2)$ and j $(m_1 - m_2)$ as edges. If no such elements exist, then $P_{ij} = 0$.

8.2 Q

$$
Q_{ij} = k_0^2 \int_\Omega \epsilon_r \vec{T}_i \cdot \vec{T}_j \; dV \tag{43}
$$

Using an identity from textbook (Jianming Jin, Chapter 8),

$$
\begin{aligned}
\vec{T}_i \cdot \vec{T}_j &= \sum_e \vec{T}_k^e \cdot \vec{T}_m^e \\
&= \frac{l_k^e l_m^e}{36} \sum_e \frac{1}{V_e^2} \Big[L_{k_1} L_{m_1} \theta_{k_2 m_2} - L_{k_1} L_{m_2} \theta_{k_2 m_1} - L_{k_2} L_{m_1} \theta_{k_1 m_2} + L_{k_2} L_{m_2} \theta_{k_1 m_1}\Big]_e
\end{aligned} \tag{44}
$$

where

$$
\boxed{\theta_{km} := b_k b_m + c_k c_m + d_k d_m \Big|_e} \tag{45}
$$

Since both $\vec{T}_i$ and $\vec{T}_j$ are linear, $\vec{T}_i \cdot \vec{T}_j$ is a quadratic polynomial in x, y and z.
It is non-zero in the tetrahedral elements e that have both i and j as global edges.

Our objective is now to find a closed form expression for the integral

$$
I(k, m) = \int_e L_k L_m dV
$$

, where the integration is over a general tetrahedron `conv` $\{\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4\}$ (`conv` refers to convex hull).

To do this integral, we perform an affine transformation so that the general tetrahedron `conv` $\{\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4\}$ transforms to the unit tetrahedron `conv` $\left\{ \begin{pmatrix} 0\\0\\0 \end{pmatrix}, \begin{pmatrix} 1\\0\\0 \end{pmatrix}, \begin{pmatrix} 0\\1\\0 \end{pmatrix}, \begin{pmatrix} 0\\0\\1 \end{pmatrix} \right\}$ (which we denote as Δ)

$$
\vec{r} = \vec{r}_1 + [J] \begin{pmatrix} u\\v\\w \end{pmatrix} \tag{46}
$$

$$
J = \begin{bmatrix} (x_2 - x_1) & (x_3 - x_1) & (x_4 - x_1) \\ (y_2 - y_1) & (y_3 - y_1) & (y_4 - y_1) \\ (z_2 - z_1) & (z_3 - z_1) & (z_4 - z_1) \end{bmatrix} \tag{47}
$$

Hence an arbitrary tetrahedron in the (x,y,z) space is transformed to the unit tetrahedron in (u,v,w) space.

Now substitute (46) in the equation for $L_i(x, y, z)$ to observe that

$$
\begin{aligned}
L_i(\vec{r}) = \tilde{L}_i(u, v, w) &= L_i(\vec{r}_1) + [L_i(\vec{r}_2) - L_i(\vec{r}_1)]u + [L_i(\vec{r}_3) - L_i(\vec{r}_1)]v + [L_i(\vec{r}_4) - L_i(\vec{r}_1)]w &(48)\\
&:= n_i + f_i u + g_i v + h_i w &(49)
\end{aligned}
$$

where we define new coefficients

$$
\boxed{n_i := L_i(\vec{r}_1) \qquad f_i := L_i(\vec{r}_2) - L_i(\vec{r}_1) \qquad g_i := L_i(\vec{r}_3) - L_i(\vec{r}_1) \qquad h_i := L_i(\vec{r}_4) - L_i(\vec{r}_1)} \tag{50}
$$

This gives us how L_i transforms under the change of variables. We also know that the infinitesimal volume dV transforms as

$$dx\ dy\ dz = |J| du\ dv\ dw \tag{51}$$

Hence

$$I(k,m) = \int_e L_k L_m dx\ dy\ dz = \int_\Delta \tilde{L}_k \tilde{L}_m |J| du\ dv\ dw \tag{52}$$

Substitute $\tilde{L}_k = (n_k + f_k u + g_k v + h_k w)$ and $\tilde{L}_m = (n_m + f_m u + g_m v + h_m w)$ in Equation (53) to find that

$$\boxed{\begin{aligned} I(k,m) := |J| \times (\frac{n_k n_m}{6} &+ \frac{1}{24}\Big[n_k(f_m + g_m + h_m) + n_m(f_k + g_k + h_k)\Big] + \frac{1}{60}\Big[f_k f_m + g_k g_m + h_k h_m\Big] \\ &+ \frac{1}{120}\Big[f_k(g_m + h_m) + f_m(g_k + h_k) + (g_k h_m + g_m h_k)\Big]) \end{aligned}} \tag{53}$$

Hint: In evaluating the integral, use the following identity

$$\int_\Delta u^p v^q w^r du\ dv\ dw = \frac{p!q!r!}{(p+q+r+3)!} \tag{54}$$

Hence

$$\boxed{Q_{ij} = k_0^2\ \frac{l_k^e l_m^e}{36} \sum_e \frac{\epsilon_r^e}{V_e^2}\Big[I(k_1,m_1)\theta_{k_2 m_2} - I(k_1,m_2)\theta_{k_2 m_1} - I(k_2,m_1)\theta_{k_1 m_2} + I(k_2,m_2)\theta_{k_1 m_1}\Big]_e} \tag{55}$$

8.3 R

$$R_{ij} = jk_0 \oint_\Gamma \sqrt{\epsilon_r} \vec{T}_i \cdot \vec{T}_j\ dS \tag{56}$$

As in the previous section,

$$\begin{aligned} \vec{T}_i \cdot \vec{T}_j &= \sum_e \vec{T}_k^e \cdot \vec{T}_m^e \\ &= \frac{l_k^e l_m^e}{36} \sum_e \frac{1}{V_e^2}\Big[L_{k_1} L_{m_1} \theta_{k_2 m_2} - L_{k_1} L_{m_2} \theta_{k_2 m_1} - L_{k_2} L_{m_1} \theta_{k_1 m_2} + L_{k_2} L_{m_2} \theta_{k_1 m_1}\Big]_e \end{aligned} \tag{57}$$

where

$$\boxed{\theta_{km} := b_k b_m + c_k c_m + d_k d_m\Big|_e} \tag{58}$$

Since both $\vec{T}_i$ and $\vec{T}_j$ are linear, $\vec{T}_i \cdot \vec{T}_j$ is a quadratic polynomial in x, y and z.
It is non-zero in the tetrahedral elements e that have both i and j as global edges.

Let the exposed triangle be

$$\Delta = \texttt{conv}\{\vec{r}_1, \vec{r}_2, \vec{r}_3\} \tag{59}$$

Our objective is now to find a closed form expression for the integral

$$B(k,m) = \int_\Delta L_k(x,y,z) L_m(x,y,z) dS \tag{60}$$

where $k, m \in \{1, 2, 3, 4\}$

Note that since $L_k L_m$ is non-zero only in the element it belongs to, the domain of integration is reduced to the exposed surface of that element. Now under the change of variables described in Appendix B, the scalar basis transforms as

$$\begin{aligned} L_k(x,y,z) &= \frac{1}{6V_e}(a_k + b_k x + c_k y + d_k z) \\ = \tilde{L}_k(\alpha, \beta) &= L_k(\vec{r}_1) + \alpha(L_k(\vec{r}_2) - L_k(\vec{r}_1)) + \beta(L_k(\vec{r}_3) - L_k(\vec{r}_1)) \\ &= p_k + q_k\alpha + r_k\beta \end{aligned} \tag{61}$$

and the same for m. Where new coeffs are introduced as

$$\boxed{p_k := L_k(\vec{r}_1) \qquad q_k := L_k(\vec{r}_2) - L_k(\vec{r}_1) \qquad r_k := L_k(\vec{r}_3) - L_k(\vec{r}_1)} \tag{62}$$

Hence

$$\int_\Delta L_k L_m dS = \int_\Delta \tilde{L}_k \tilde{L}_m dS_\alpha = 2 \text{ Area}(\Delta) \int_{\text{unit tri}} \tilde{L}_k \tilde{L}_m \; d\alpha \; d\beta \tag{63}$$

Now note the identity

$$\int_{\text{unit tri}} \alpha^{c_1} \beta^{c_2} d\alpha \; d\beta = \frac{c_1! c_2!}{(c_1 + c_2 + 2)!} \tag{64}$$

Hence

$$\boxed{B(k,m) = \text{Area}(\Delta) \left[p_k p_m + \frac{1}{3}\Big(p_k(q_m + r_m) + p_m(q_k + r_k)\Big) + \frac{1}{6}(q_k q_m + r_k r_m) + \frac{1}{12}(q_k r_m + q_m r_k) \right]} \tag{65}$$

Hence we have

$$\boxed{R_{ij} = jk_0 \, \frac{l_k^e l_m^e}{36} \sum_e \frac{\sqrt{\epsilon_r^e}}{V_e^2} \Big[B(k_1, m_1)\theta_{k_2 m_2} - B(k_1, m_2)\theta_{k_2 m_1} - B(k_2, m_1)\theta_{k_1 m_2} + B(k_2, m_2)\theta_{k_1 m_1} \Big]_e} \tag{66}$$

8.4 S

$$S_{ij} = jk_0 \int_\Delta \sqrt{\epsilon_r} (\vec{T}_i \cdot \hat{n})(\vec{T}_j \cdot \hat{n}) \; dS \tag{67}$$

Let the exposed triangle be

$$\Delta = \texttt{conv}\{\vec{r}_1, \vec{r}_2, \vec{r}_3\} \tag{68}$$

Note that

$$(\vec{T}_i \cdot \hat{n})(\vec{T}_j \cdot \hat{n}) = \sum_e (\vec{T}_k^e \cdot \hat{n})(\vec{T}_m^e \cdot \hat{n}) \tag{69}$$

We know from a previous section that

$$\vec{T}_k = l_k(L_{k_1} \nabla L_{k_2} - L_{k_2} \nabla L_{k_1}) \tag{70}$$

Let $\hat{n} = (n_x, n_y, n_z)$ for the exposed triangle. Define

$$\boxed{\Psi_k = b_k n_x + c_k n_y + d_k n_z \Big|_e} \tag{71}$$

Then

$$\vec{T}_k \cdot \hat{n} = \frac{l_k}{36V_e^2}\Big[(a_{k_1}\Psi_{k_2} - a_{k_2}\Psi_{k_1}) + (b_{k_1}\Psi_{k_2} - b_{k_2}\Psi_{k_1})x + (c_{k_1}\Psi_{k_2} - c_{k_2}\Psi_{k_1})y + (d_{k_1}\Psi_{k_2} - d_{k_2}\Psi_{k_1})z\Big]$$
$$:= \frac{l_k}{36V_e^2}F_k(x,y,z) \tag{72}$$

$$\boxed{F_k(x,y,z) = \Big[(a_{k_1}\Psi_{k_2} - a_{k_2}\Psi_{k_1}) + (b_{k_1}\Psi_{k_2} - b_{k_2}\Psi_{k_1})x + (c_{k_1}\Psi_{k_2} - c_{k_2}\Psi_{k_1})y + (d_{k_1}\Psi_{k_2} - d_{k_2}\Psi_{k_1})z\Big]} \tag{73}$$

Under the change of variables defined in Appendix B, this function transforms as

$$\boxed{\tilde{F}_k(\alpha,\beta) = u_k + v_k\alpha + w_k\beta} \tag{74}$$

where new coeffs are introduced as

$$\boxed{u_k := F_k(\vec{r}_1) \qquad v_k := F_k(\vec{r}_2) - F_k(\vec{r}_1) \qquad w_k := F_k(\vec{r}_3) - F_k(\vec{r}_1)} \tag{75}$$

Now we can define a two-edge integral $\zeta(k,m)$ as follows and note that

$$\zeta(k,m) = \int_\Delta F_k F_m dS = \int_\Delta \tilde{F}_k\tilde{F}_m dS_\alpha = 2\ \text{Area}(\Delta)\int_{\text{unit tri}} \tilde{F}_k\tilde{F}_m\ d\alpha\ d\beta \tag{76}$$

$$\boxed{\zeta(k,m) = \text{Area}(\Delta)\left[u_k u_m + \frac{1}{3}\Big(u_k(v_m+w_m) + u_m(v_k+w_k)\Big) + \frac{1}{6}(v_k v_m + w_k w_m) + \frac{1}{12}(v_k w_m + v_m w_k)\right]} \tag{77}$$

Hence

$$\boxed{S_{ij} = jk_0\ \frac{l_k^e l_m^e}{1296}\sum_e \frac{\sqrt{\epsilon_r^e}}{V_e^4}\ \zeta(k,m)} \tag{78}$$

8.5 b

$$b(\vec{T}) := \begin{cases} \oint_\Gamma \left[-jk_0\sqrt{\epsilon_r}\left(\vec{T}\cdot(\hat{n}\times(\hat{n}\times\vec{E}_{inc})\right) - \vec{T}\cdot\left(\hat{n}\times(\nabla\times\vec{E}_{inc})\right)\right] dS, & \vec{J}=0 \\ -j\omega\mu_0\int_\Omega \vec{T}\cdot\vec{J}\,dV, & \vec{J}\neq 0 \end{cases} \tag{79}$$

Let us first evaluate the $\vec{J}=0$ case.

The incident field is a plane wave, polarized along $\hat{E}$, given by

$$\vec{E}_{inc} = e^{-j\vec{k}_0\cdot\vec{r}}\hat{E} \tag{80}$$

Upon substituting this in (79) and simplifying, we get

$$b(\vec{T}) = jk_0\int_\Delta dS\; e^{-j\vec{k}_0\cdot\vec{r}}\left[(\vec{T}\cdot\hat{E})\left(\sqrt{\epsilon_r}-(\hat{k}_0\cdot\hat{n})\right) - (\hat{n}\cdot\hat{E})\left(\vec{T}\cdot(\sqrt{\epsilon_r}\hat{n}-\hat{k}_0)\right)\right] \tag{81}$$

Note that the domain of integration is reduced to the exposed triangle of the element in which $\vec{T}$ is non-zero.

We approximate the integral as follows. Let $\vec{r}_G$ denote the coordinates of the centroid of the exposed triangle. Then

$$\boxed{b(\vec{T}) \approx \text{Area}(\Delta)\; jk_0\; e^{-j\vec{k}_0\cdot\vec{r}_G}\left[(\vec{T}(\vec{r}_G)\cdot\hat{E})\left(\sqrt{\epsilon_r}-(\hat{k}_0\cdot\hat{n})\right) - (\hat{n}\cdot\hat{E})\left(\vec{T}(\vec{r}_G)\cdot(\sqrt{\epsilon_r}\hat{n}-\hat{k}_0)\right)\right]} \tag{82}$$

We may choose the following direction of propogation defined by fixed angles (θ,ϕ)

$$\hat{k}_0 = -(\sin\theta\cos\phi,\;\; \sin\theta\sin\phi,\;\; \cos\theta) \tag{83}$$

Polarization is perpendicular to this direction, and we may choose

$$\hat{E} = (\cos\theta\cos\phi,\;\; \cos\theta\sin\phi,\;\; -\sin\theta) \tag{84}$$

Remember that this not the only choice, any direction perpendicular to $\hat{k}_0$ will do.

Let the outward unit normal vector at the exposed triangle be

$$\hat{n} = (n_x,\;\; n_y,\;\; n_z) \tag{85}$$

To simplify (82), we need to introduce intermediate variables. Define

$$\boxed{\xi_j = b_j\cos\theta\cos\phi + c_j\cos\theta\sin\phi - d_j\sin\theta} \tag{86}$$

Also define

$$\boxed{\Upsilon_j = b_j(\sqrt{\epsilon_r}n_x+\sin\theta\cos\phi) + c_j(\sqrt{\epsilon_r}n_y+\sin\theta\sin\phi) + d_j(\sqrt{\epsilon_r}n_z+\cos\theta)} \tag{87}$$

Then

$$\boxed{\begin{aligned} \vec{T}(\vec{r}_G)\cdot\hat{E} &= \frac{l}{36V^2}\left[(a_1\xi_2-a_2\xi_1)+(b_1\xi_2-b_2\xi_1)x_G+(c_1\xi_2-c_2\xi_1)y_G+(d_1\xi_2-d_2\xi_1)z_G\right] \\ \vec{T}\cdot(\sqrt{\epsilon_r}\hat{n}-\hat{k}_0) &= \frac{l}{36V^2}\left[(a_1\Upsilon_2-a_2\Upsilon_1)+(b_1\Upsilon_2-b_2\Upsilon_1)x_G+(c_1\Upsilon_2-c_2\Upsilon_1)y_G+(d_1\Upsilon_2-d_2\Upsilon_1)z_G\right] \end{aligned}}$$

(88)

(89)

And

$$\boxed{\begin{aligned}
\hat{n}\cdot\hat{E} &= n_x\cos\theta\cos\phi + n_y\cos\theta\sin\phi - n_z\sin\theta && (90)\\
(\sqrt{\epsilon_r} - \hat{k}_0\cdot\hat{n}) &= \sqrt{\epsilon_r} + n_x\sin\theta\cos\phi + n_y\sin\theta\sin\phi + n_z\cos\theta && (91)\\
jk_0 e^{-j\vec{k}_0\cdot\vec{r}_G} &= k_0\left(-\sin\left(k_0\tau\right) + j\cos\left(k_0\tau\right)\right) && (92)\\
\tau &= x_G\sin\theta\cos\phi + y_G\sin\theta\sin\phi + z_G\cos\theta && (93)
\end{aligned}}$$

All these expressions can be substituted in (82)

9 Far-field using Huygen's Principle

The Helmholtz equation in the region outside the scatterer takes the form

$$\nabla \times (\nabla \times \vec{E}) - k^2 \vec{E} = Q(r) \tag{94}$$

The free space dyadic Green's function $\overleftrightarrow{G}(r, r')$ satisfies

$$\nabla \times (\nabla \times \overleftrightarrow{G}) - k^2 \overleftrightarrow{G} = \overleftrightarrow{I}\, \delta(r - r') \tag{95}$$

Take a dot product of Equation (94) with $\overleftrightarrow{G}$ and Equation (95) with $\vec{E}$, subtract them, and volume integrate (over the domain outside the scatterer, denoted V_1) on both sides. The RHS would then be the scattered field. Hence, we have

$$\vec{E}_{scat}(r') = \pm \int_{V_1} \left[(\nabla \times (\nabla \times \overleftrightarrow{G})) \cdot \vec{E} - \overleftrightarrow{G} \cdot (\nabla \times (\nabla \times \vec{E})) \right] dV \tag{96}$$

Note the following identity [2] that turns the volume integral into a surface integral on the surface of the scatterer (denoted R)

$$\int_{V} \left[(\nabla \times (\nabla \times \overleftrightarrow{Q})) \cdot \vec{P} - \overleftrightarrow{Q} \cdot (\nabla \times (\nabla \times \vec{P})) \right] dV = - \oint_{R} \left[\overleftrightarrow{Q} \cdot \hat{n} \times (\nabla \times \vec{P}) + (\nabla \times \overleftrightarrow{Q}) \cdot (\hat{n} \times \vec{P}) \right] dS \tag{97}$$

Hence, we have

$$\boxed{\vec{E}_{scat}(r') = \pm \oint_{R} \left[\overleftrightarrow{G} \cdot \hat{n} \times (\nabla \times \vec{E}) + (\nabla \times \overleftrightarrow{G}) \cdot (\hat{n} \times \vec{E}) \right] dS} \tag{98}$$

The overall plus or minus exists depending on how we absorb $Q(r)$ as incident field. Here, surface integration is over unprimed coordinates (r) on the surface of the scatterer (R). The far field point is r'. Now, from FEM, we get field coefficients u_m for <u>edges belonging to surface elements</u>. The sum index m in the following equation is only over such edges.

$$\vec{E}_{scat}(r') = \pm \sum_{m} u_m \oint_{R} \left[\overleftrightarrow{G} \cdot \hat{n} \times (\nabla \times \vec{T}_m) + (\nabla \times \overleftrightarrow{G}) \cdot (\hat{n} \times \vec{T}_m) \right] dS \tag{99}$$

In the far-field limit, the 3D dyadic Green's function takes the form [2]

$$\overleftrightarrow{G} \approx (\overleftrightarrow{I} - \hat{r'}\hat{r'}) \frac{e^{-jk|r-r'|}}{4\pi |r'|} \tag{100}$$

Here, $\hat{r'}\hat{r'}$ represents the outer product of the unit position vector corresponding to r' with itself. The curl of the dyadic green's function is given by [2]

$$\nabla \times \overleftrightarrow{G} = \begin{bmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix} \frac{e^{-jk|r-r'|}}{4\pi |r'|} \tag{101}$$

Simplifying Equation (101) in the far-field approximation, we get

$$\nabla \times \overleftrightarrow{G} \approx \begin{bmatrix} 0 & -z' & y' \\ z' & 0 & -x' \\ -y' & x' & 0 \end{bmatrix} \frac{-jk}{4\pi |r'|^2} e^{-jk|r-r'|} \tag{102}$$

The curl of our vector basis function is given by

$$\nabla \times \vec{T} = \frac{l}{18V^2}(c_1 d_2 - c_2 d_1, d_1 b_2 - d_2 b_1, b_1 c_2 - b_2 c_1) := \frac{l}{18V^2}(\beta_1, \beta_2, \beta_3) \tag{103}$$

Then

$$\hat{n} \times (\nabla \times \vec{T}) = \frac{l}{18V^2}\begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ n_x & n_y & n_z \\ \beta_1 & \beta_2 & \beta_3 \end{vmatrix} := \frac{l}{18V^2}(\alpha_1, \alpha_2, \alpha_3) \tag{104}$$

Using the expressions in equations (104) and (100) in the first term of the scattered field integral equation (99), after simplifications, we have

$$\Rightarrow \overleftrightarrow{G} \cdot \hat{n} \times (\nabla \times \vec{T}) = \frac{l}{72\pi V^2}\frac{\mathbf{M}\,|\alpha\rangle}{|r'|^3}e^{-jk|r-r'|} \tag{105}$$

where

$$\boxed{\mathbf{M} := \begin{bmatrix} y'^2 + z'^2 & -x'y' & -x'z' \\ -x'y' & x'^2 + z'^2 & -y'z' \\ -x'z' & -y'z' & x'^2 + y'^2 \end{bmatrix} \qquad |\alpha\rangle := \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix}} \tag{106}$$

where

$$\alpha_1 := (n_y\beta_3 - n_z\beta_2) \qquad \alpha_2 := (n_z\beta_1 - n_x\beta_3) \qquad \alpha_3 := (n_x\beta_2 - n_y\beta_1) \tag{107}$$

$$\beta_1 := (c_1 d_2 - c_2 d_1) \qquad \beta_2 := (d_1 b_2 - d_2 b_1) \qquad \beta_3 := (b_1 c_2 - b_2 c_1) \tag{108}$$

Now

$$\hat{n} \times \vec{T} := \frac{l}{36V^2}\begin{pmatrix} \gamma_x(r) \\ \gamma_y(r) \\ \gamma_z(r) \end{pmatrix} := \frac{l}{36V^2}\,|\gamma(r)\rangle \tag{109}$$

Using the expressions in equations (109) and (102) in the second term of the scattered field integral equation (99), after simplifications, we have

$$\Rightarrow (\nabla \times \overleftrightarrow{G}) \cdot (\hat{n} \times \vec{T}) = \frac{l}{144\pi V^2}\frac{-jk\mathbf{N}\,|\gamma(r)\rangle}{|r'|^2}e^{-jk|r-r'|} \tag{110}$$

where

$$\boxed{\mathbf{N} = \begin{bmatrix} 0 & -z' & y' \\ z' & 0 & -x' \\ -y' & x' & 0 \end{bmatrix} \qquad |\gamma(r)\rangle = \begin{pmatrix} \gamma_x(r) \\ \gamma_y(r) \\ \gamma_z(r) \end{pmatrix}} \tag{111}$$

where

$$\boxed{\begin{aligned} \gamma_x(r) &:= 6V\Big[n_y(d_2 L_1(r) - d_1 L_2(r)) - n_z(c_2 L_1(r) - c_1 L_2(r))\Big] \\ \gamma_y(r) &:= 6V\Big[n_z(b_2 L_1(r) - b_1 L_2(r)) - n_x(d_2 L_1(r) - d_1 L_2(r))\Big] \\ \gamma_z(r) &:= 6V\Big[n_x(c_2 L_1(r) - c_1 L_2(r)) - n_y(b_2 L_1(r) - b_1 L_2(r))\Big] \end{aligned}} \tag{112}$$

Using the results in equations (105) and (110) in the scattered field integral equation (99), we finally have

$$\boxed{\vec{E}_{scat}(r') \approx \pm\frac{\exp\left(-jk_0\sqrt{\epsilon_r}|r'|\right)}{72\pi|r'|^2}\sum_m \left[\frac{u_m l_m \Delta_e}{V_e^2}\left(\frac{\mathbf{M}\,|\alpha\rangle_m}{|r'|} - \frac{jk_0\sqrt{\epsilon_r}}{2}\mathbf{N}\,|\gamma(r_G)\rangle_m\right)\right]} \tag{113}$$

Here Δ_e is the area of the exposed surface of a surface-element e, V_e is its volume, $r_G = (r_1 + r_2 + r_3)/3$ is the position vector of the centroid of the exposed triangle.

Equation (113) is a neat result. Physically, it can be interpreted as a linear superposition of the fields created by secondary point-sources located at the centroids of exposed triangles on the surface of the scatterer (a sphere in our case). Notice that there is a $1/|r'|^2$ outside. But also note that $\mathbf{M}/|r'|$ and $\mathbf{N}$ have entries that linear in the coordinates of r'. So effectively, we can interpret the result as a linear superposition of secondary point-sources.

10 Mie scattering Formulation

10.1 Vector function Formalism

For Mie scattering formulation, we refer to these sources [3, 4]. Consider a linear, isotropic, homogeneous medium in the absence of source, any field $\vec{C}$ must satisfy the homogeneous wave equation as follows:

$$\nabla^2 \vec{C} + k^2 \vec{C} = 0 \tag{114}$$

This vector differential equation can be projected along the unit vectors, of a generic reference system, becoming a system of three scalar differential equations. However, such a system is not easy to solve in most of the coordinate systems. While the solution of the vector Helmholtz equation is not a simple task in several coordinate systems, it is easy to solve the scalar Helmholtz equation:

$$\nabla^2 \psi + k^2 \psi = 0 \tag{115}$$

At this point we define the vector harmonics as follows:

$$\vec{M} = \nabla \times (\vec{r}\psi_{m,n})$$

$$\vec{N} = \frac{\nabla \times \vec{M}}{k}$$

Recalling the relation between the magnetic potential and the electric field and applying the Maxwell equations, we can write the following expressions of the electric and magnetic fields:

$$\vec{E} = \sum_{n=0}^{\infty} (a_n \vec{M}_n + b_n \vec{N}_n) \tag{116}$$

$$\vec{H} = \frac{k}{j\omega\mu} \sum_{n=0}^{\infty} (a_n \vec{N}_n + b_n \vec{M}_n) \tag{117}$$

Mie's solution to Maxwell's equations describes the scattering of an electromagnetic plane wave by a homogeneous sphere. Mie scattering results in the case when the particle size is comparable to the wavelength of the wave incident on it.

In spherical coordinates,Helmholtz equation is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2 \partial \Psi}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \Psi}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 \Psi}{\partial \psi^2} + k^2 \Psi = 0 \tag{118}$$

We use the method of separation of variables

$$\Psi = R(r)H(\theta)\Phi(\phi)$$

Substituting this into Eq 103, dividing by Ψ, and multiplying by $r^2 \sin^2\theta$, we obtain

$$\frac{\sin^2\theta}{R}\frac{\partial}{dr}\left(\frac{r^2 dR}{dr}\right) + \frac{\sin\theta}{H}\frac{d}{d\theta}\left(\sin\theta \frac{dH}{d\theta}\right) + \frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} + k^2 r^2 \sin^2\theta = 0 \tag{119}$$

The ϕ dependence is now separated and we let

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2$$

Substitution of this into the preceding equation and division by $\sin^2\theta$ yields

$$\frac{1}{R}\frac{\partial}{dr}\left(\frac{r^2 dR}{dr}\right) + \frac{1}{H\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dH}{d\theta}\right) - \frac{m^2}{\sin^2\theta} + k^2r^2 = 0 \tag{120}$$

This separates r and θ dependence. Let

$$\frac{1}{H\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dH}{d\theta}\right) - \frac{m^2}{\sin^2\theta} = -n(n+1) \tag{121}$$

With this choice, the preceding equation becomes

$$\frac{1}{R}\frac{\partial}{dr}\left(\frac{r^2 dR}{dr}\right) - n(n+1) + k^2r^2 = 0 \tag{122}$$

Collecting the above results, we have the trio of separated equations.

$$\frac{\partial}{dr}\left(\frac{r^2 dR}{dr}\right) - (n(n+1) + k^2r^2)R = 0 \tag{123}$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} + m^2 = 0 \tag{124}$$

$$\frac{1}{H\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dH}{d\theta}\right) - \frac{m^2}{\sin^2\theta} = -n(n+1) \tag{125}$$

The ϕ equation is the familiar harmonic equation giving rise to solutions $h(m\phi)$. The R equation is closely related to Bessel's equation. Its solutions are called spherical Bessel functions, denoted by $b_n(kr)$, which are related to ordinary Bessel functions by

$$z_n(kr) = \sqrt{\frac{\pi}{2kr}}Z_{n+\frac{1}{2}}(kr)$$

where $z_n(kr)$ can be $j_n(kr), n_n(kr), h_n^{(1)}(kr), h_n^{(2)}(kr)$. The θ equation is related to Legendre's equation, and its solutions are called associated Legendre functions. We shall denote solutions in general by $L_n^m(\cos\theta)$.Commonly used solutions are

$$L_n^m(\cos\theta) \approx P_n^m(\cos\theta), Q_n^m(\cos\theta) \tag{126}$$

where $P_n^m(\cos\theta)$ are the associated Legendre functions of the first kind and $Q_n^m(\cos\theta)$ are the associated Legendre functions of the second kind.

We can now form product solutions to the Helmholtz equation as

$$\Psi_{m,n} = z_n(kr)L_n^m(\cos\theta)h(m\phi) \tag{127}$$

These are elementary wave functions for the spherical coordinate system.

We can form general solutions to the Helmholtz equation by forming a linear combination of elementary wave functions.

1. As ϕ is 2π periodic ,if a single valued ψ in the range from 0 to 2π is desired,then choose $h(m\phi)$ to be the linear combination of $\sin m\phi$ and $\cos m\phi$ or $e^{jm\phi}$ and $e^{-jm\phi}$ with m being an integer.

2. Study of solution to the assosiated Legendre equation shows that all solutions have singularities at $\theta = 0$ $\theta = \pi$ except $P_n^m(\cos\theta)$ with n being an integer.For ψ to be finite in the range $0 \leq \theta \leq \pi$

$$L_n^m(\cos\theta) = P_n^m(\cos\theta)$$

3. For radial part,spherical Bessel function solutions are $J_{n+1/2}(kr)$ and $N_{n+1/2}(kr)$ which, means that the solutions for $R(r)$ are the spherical Bessel and Neumann functions,$j_n(kr)$ and $n_n(kr)$ defined by

$$\boxed{j_n(kr) = \sqrt{\frac{\pi}{2kr}} J_{n+\frac{1}{2}}(kr)}$$

$$\boxed{n_n(kr) = \sqrt{\frac{\pi}{2kr}} N_{n+\frac{1}{2}}(kr)}$$

From now one we will assume that the solution is finite at the origin, which rules out $n_n(kr)$,and so

$$\boxed{R(r) = j_n(kr)}$$

Hence to represent a finite field inside the sphere,elementary wave functions will be

$$\boxed{\psi_{m,n} = j_n(kr)P_n^m(\cos\theta)e^{jm\phi}}$$

To represent the field ,outside the sphere,we must choose outward-travelling wave

$$\boxed{\psi_{m,n} = h_n^{(2)}(kr)P_n^m(\cos\theta)e^{jm\phi}}$$

Any linear combination of $j_n(kr)$ and $n_n(kr)$ is also a solution to 104. Two such combinations deserve special attention, the spherical Bessel functions of the third kind (sometimes called spherical Hankel functions):

$$\boxed{h_n^{(1)}(kr) = j_n(kr) + n_n(kr)}$$

$$\boxed{h_n^{(2)}(kr) = j_n(kr) - n_n(kr)}$$

As Φ can be written as linear combinations of real sine and cosine function with m from $-\infty$ to ∞

$$\Phi(\phi) = \cos m\phi + \sin m\phi$$

Substituting the values we get,

$$\boxed{\Psi_{e,m,n} = j_n(kr)P_n^m(\cos\theta)\cos m\phi} \tag{128}$$

$$\boxed{\Psi_{o,m,n} = j_n(kr)P_n^m(\cos\theta)\sin m\phi} \tag{129}$$

where subscript e and o denotes even and odd solutions. Both the solutions are linearly independent.

Any function that satisfies the scalar wave equation in spherical polar coordinates may be expanded as an infinite series. The vector spherical harmonics generated by $\psi_{e,m,n}$ and $\psi_{o,m,n}$ will represent the electromagnetic field in terms of wave functions. Let us formulate the equations for M and N ($\rho = kr$)

$$M_{m,n}(r) = \frac{jm}{\sin\theta} z_n(kr)P_n^m(\cos\theta)e^{jm\phi}\hat{\theta} - z_n(kr)\frac{d}{d\theta}\left(P_n^m(\cos\theta)\right)e^{jm\phi}\hat{\phi} \tag{130}$$

$$N_{mn}(r) = \frac{z_n(kr)}{kr} n(n+1) P_n^m(\cos\theta) e^{jm\phi}\hat{r} + \frac{1}{kr}\frac{\partial}{\partial r}\left(r z_n(kr)\right) \frac{\partial P_n^m(\cos\theta)}{\partial\theta} e^{jm\phi}\hat{\theta} + \frac{1}{kr}\frac{\partial}{\partial r}\left(r z_n(kr)\right) \frac{jm}{\sin\theta} P_n^m(\cos\theta) e^{jm\phi}\hat{\phi} \quad (131)$$

At this point, three important vector functions can be introduced:

$$\boxed{m_{mn}(\theta,\phi) = e^{jm\phi}[j\pi_{mn}(\cos\theta)\hat{\theta} - \tau_{mn}(\cos\theta)\hat{\phi}]}$$

$$\boxed{n_{mn}(\theta,\phi) = e^{jm\phi}[\tau_{mn}(\cos\theta)\hat{\theta} + j\pi_{mn}(\cos\theta)\hat{\phi}]}$$

$$\boxed{p_{mn} = e^{jm\phi} n(n+1) P_n^m(\cos\theta)\hat{r}}$$

where π_{mn} and τ_{mn} are called scalar tesseral functions, related to the associated Legendre function as

$$\pi_{mn}(\theta) = m\frac{P_n^m(\cos\theta)}{\sin\theta}$$

$$\tau_{mn}(\theta) = \frac{dP_n^m(\cos\theta)}{d\theta}$$

Any solution to the field equations can now be expanded in an infinite series of functions. Thus, armed with vector harmonics, we are ready to attack the problem of scattering by an arbitrary sphere.

11 Expansion of a plane wave in vector spherical harmonics

The problem with which we are concerned is the scattering of a general plane wave, written in spherical polar coordinates as

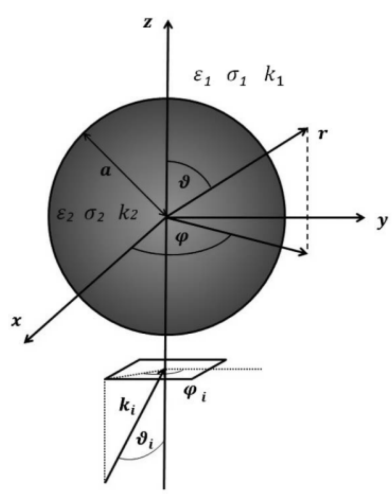

Figure 3: Representation of a plane wave incident on a sphere

Consider a general elliptic plane polarised wave incident on the sphere as shown in Figure 3

$$E_i(r) = e_{pol} e^{-jk_i.r} = (E_{\theta_i}\hat{\theta}_i + E_{\phi_i}\hat{\phi}_i) e^{-jk_i.r} \quad (132)$$

$$\hat{e}_x = \sin\theta\cos\phi\hat{e}_r + \cos\theta\cos\phi\hat{e}_\theta - \sin\phi\hat{e}_\phi \tag{133}$$

where e_{pol} is the polarization vector of the plane wave. The vectors $\hat{\theta}_i$ and $\hat{\phi}_i$ are the unit vectors of the local spherical coordinate frame with respect to the wave vector of the plane wave. where

$$k_i = k_1\hat{k}_i = k_1(\sin\theta_i\cos\phi_i\hat{x} + \sin\theta_i\sin\phi_i\hat{y} + \cos\theta_i\hat{z}) \tag{134}$$

$$\phi_i = \frac{\hat{z}\times\hat{k}_i}{|\hat{z}\times\hat{k}_i|} = -\sin\phi_i\hat{x} + \cos\phi_i\hat{y} \tag{135}$$

$$\theta_i = \hat{\phi}\times\hat{k}_i = \cos\theta_i\cos\phi_i\hat{x} + \cos\theta_i\sin\phi_i\hat{y} - \sin\theta_i\hat{z} \tag{136}$$

The elevation angle θ_i is the angle between the wave vector and the z-axis, while the azimuthal angle ϕ_i is the angle between the projection of the wave vector on the x, y plane and the x axis. The incident plane wave can be expanded in spherical harmonics as follows:

$$E_i(r) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}[a_{mn}M_{mn}^{(1)}(r) + b_{mn}N_{mn}^{(1)}(r)] \tag{137}$$

with

$$\boxed{a_{mn} = (-1)^m j^n \frac{2n+1}{n(n+1)}\frac{(n-m)!}{(n+m)!}e_{pol}.m_{mn}^*(\theta_i,\phi_i)} \tag{138}$$

$$\boxed{b_{mn} = (-1)^m j^{n-1} \frac{2n+1}{n(n+1)}\frac{(n-m)!}{(n+m)!}e_{pol}.n_{mn}^*(\theta_i,\phi_i)} \tag{139}$$

Here superscript (1) in the vector harmonics indicates that the radial dependence follows the spherical Bessel function of the first kind,$j_n(kr)$.

The scattered field can be expanded in spherical vector wave functions as well:

$$E_s(r) = \sum_{n=1}^{\infty}\sum_{m=-n}^{n}[c_{mn}M_{mn}^{(3)}(r) + d_{mn}N_{mn}^{(3)}(r)] \tag{140}$$

The superscript (3) in the vector harmonics indicates that the radial dependence follows the spherical Bessel function of the third kind, i.e., the spherical Hankel function of the first type, typical for progressive waves. The coefficients c_{mn} and d_{mn} in equation (116) are the unknowns of the problem and they would be determined applying the boundary conditions, i.e., the cancellation of the tangential components of the electric fields on the sphere's surface:

$$(E_i + E_s)\times\hat{r} = 0 \qquad\qquad for r = a \tag{141}$$

Finally after applying boundary conditions and solving we get

$$\boxed{c_{mn} = -a_{mn}\frac{j_n(k_1a)}{h_n^{(1)}(k_1a)}} \tag{142}$$

$$\boxed{d_{mn} = -b_{mn}\frac{j_n^{'}(k_1a)}{h_n^{(1)'}(k_1a)}} \tag{143}$$

These coefficients are known as Mie scattering coefficients for a PEC sphere.

A Finding surface integrals over the arbitrary triangle in 3D (Projection Approach)

Let the equation of the plane of triangle formed by three points (x_1, y_1, z_1), (x_2, y_2, z_2), (x_3, y_3, z_3) be given by

$$z = \gamma_0 + \gamma_1 x + \gamma_2 y \tag{144}$$

Now the surface integral in 3D can be transformed into a 2D integral by taking its projection onto x-y plane and solving it over the surface Γ'. Correspondingly the surface element dS gets transformed into $dS' = 1/cos(\theta)dS$, where θ is the angle that the normal of the plane makes with the z-axis.

$$\begin{aligned} \int_\Gamma f(x,y,z)dS &= \int_{\Gamma'} f(x,y,\gamma_0 + \gamma_1 x + \gamma_2 y)dS' \\ &= \sqrt{1+\gamma_1^2+\gamma_2^2} \int_{\Gamma'} f(x,y,\gamma_0 + \gamma_1 x + \gamma_2 y)\, dS \end{aligned} \tag{145}$$

Now the arbitrary triangle in 2D is transformed into a unit triangle with vertices at (0,0), (0,1) and (1,1) through a change of coordinates $(x, y) \to (u, v)$. Therefore the final expression for evaluating the integral can be written as

$$\int_\Gamma f(x,y,z)dS = J\sqrt{1+\gamma_1^2+\gamma_2^2} \int_0^1 \int_0^{1-u} f(u,v)\, dv\, dv \tag{146}$$

where J is the Jacobian given by

$$J = \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} \end{vmatrix} \tag{147}$$

B Simplest approach

Again, in the (x,y,z) space, consider the triangle

$$\Gamma = \mathtt{conv}\{\vec{r_1}, \vec{r_2}, \vec{r_3}\} \tag{148}$$

where we would like to evaluate the integral

$$I = \int_\Gamma f(x,y,z)dS \tag{149}$$

Define

$$\vec{u} = (\vec{r_2} - \vec{r_1}) \quad \& \quad \vec{v} = (\vec{r_3} - \vec{r_1}) \tag{150}$$

Then an arbitrary point on or inside Γ can be written as

$$\vec{r} = \vec{r_1} + \alpha\vec{u} + \beta\vec{v} \tag{151}$$

with the constraints

$$\Gamma' : \quad \alpha, \beta \geq 0 \quad \& \quad (\alpha + \beta) \leq 1 \tag{152}$$

Since an arbitrary area element is a parallelogram with area element

$$dS_\alpha = |u||v| \sin\theta \; d\alpha \; d\beta \tag{153}$$

the integral transforms as

$$\int_\Gamma f(x,y,z)\; dS \longrightarrow |u||v|\sin\theta \int_{\Gamma'} \tilde{f}(\alpha,\beta)\; d\alpha\; d\beta \tag{154}$$

where θ is the angle between $\vec{u}$ and $\vec{v}$. Also note that

$$|u||v|\sin\theta = 2\text{Area}(\Gamma) \tag{155}$$

hence giving us a simple prescription.

C Rotation Approach

Suppose that the unit normal vector at the exposed triangle Γ is given by

$$\hat{n} = l\hat{x} + m\hat{y} + n\hat{z} \tag{156}$$

Suppose ϕ is the angle $\hat{n}$ makes with the Z axis, and θ is the angle its projection makes with the X axis. From simple trigonometry,

$$\cos\phi = n \qquad \sin\phi = \sqrt{l^2 + m^2} \tag{157}$$

And

$$\cos\theta = \frac{m}{\sqrt{l^2 + m^2}} \qquad \sin\theta = \frac{l}{\sqrt{l^2 + m^2}} \tag{158}$$

The rotation matrix which can transform $\hat{n}$ to $\hat{z}$ ($J\hat{n} = \hat{z}$) is given by

$$J = R_x(\phi)R_z(\theta) = \frac{1}{\sqrt{l^2 + m^2}} \begin{bmatrix} m & -l & 0 \\ nl & mn & -(l^2 + m^2) \\ l\sqrt{l^2 + m^2} & m\sqrt{l^2 + m^2} & n\sqrt{l^2 + m^2} \end{bmatrix} \tag{159}$$

Equivalently, the (x, y, z) space is transformed by J^T to, say, the (u, v, w) space. Then

$$dS_{(x,y,z)} = |J^T| \, dS_{(u,v,w)} \tag{160}$$

and hence the integral can be evaluated on a plane parallel to the XY plane.

D Dyadic Green's function

Consider the free space scalar Green's function in 3D.

$$g(\vec{r}, \vec{r}') = \frac{1}{4\pi} \frac{e^{-jk|\vec{r} - \vec{r}'|}}{|\vec{r} - \vec{r}'|} \tag{161}$$

The expression for the dyadic Green's function of free-space $\bar{\bar{G}}(\vec{r}, \vec{r}')$ is given by

$$\bar{\bar{G}}(\bar{r}, \bar{r}') = \left(1 + \frac{1}{k^2}\nabla\nabla\cdot\right) g(\bar{r}, \bar{r}')(\hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}) \tag{162}$$

The dyadic Green's function can be represented in matrix form as follows:

$$\bar{\bar{G}}(\bar{r}, \bar{r}') = \begin{pmatrix} k^2 + \frac{\partial^2}{\partial x^2} & \frac{\partial^2}{\partial x \partial y} & \frac{\partial^2}{\partial x \partial z} \\ \frac{\partial^2}{\partial y \partial x} & k^2 + \frac{\partial^2}{\partial y^2} & \frac{\partial^2}{\partial y \partial z} \\ \frac{\partial^2}{\partial z \partial x} & \frac{\partial^2}{\partial z \partial y} & k^2 + \frac{\partial^2}{\partial z^2} \end{pmatrix} \frac{e^{-jk|\vec{r} - \vec{r}'|}}{4\pi k^2 |\vec{r} - \vec{r}'|} \tag{163}$$

Through some algebra, it can be further simplified to

$$\bar{\bar{G}}(r, r') = \left(\left(\frac{3}{k^2R^2} - \frac{3i}{kR} - 1\right)\hat{R}\hat{R} + \left(\frac{3}{k^2R^2} - \frac{3i}{kR} - 1\right)\bar{\bar{I}}\right) g(R) \tag{164}$$

where $R = \vec{r} - \vec{r}'$, $\bar{\bar{I}} = \hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z}$ is the unit dyad and $g(R)$ is the scalar Green's function given by Eq. 161.

In the Cartesian coordinate system, we have the following simplification

$$\nabla \times \bar{\bar{G}}(\bar{r}, \bar{r}') = \begin{pmatrix} 0 & -\frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & -\frac{\partial}{\partial x} \\ -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{pmatrix} \frac{e^{-jk|\vec{r} - \vec{r}'|}}{4\pi|\vec{r} - \vec{r}'|} \tag{165}$$

E Associated Legendre Functions and Spherical Bessel function

The associated Legendre function is defined as

$$P_n^m(x) = \frac{(-1)^m}{2^n n!}((1-x^2))^{\frac{m}{2}} \frac{d^{n+m}}{dx^{n+m}}(x^2-1)^n \tag{166}$$

for$m = 0, 1, 2..., n$

The spherical Bessel function of the first kind denoted

$$j_n(z) = (-1)^n z^n (\frac{d}{zdz})^n \frac{\sin z}{z} \tag{167}$$

The derivatives follow from the spherical Bessel functions themselves, namely

$$[zj_n(z)]' = zj_{n-1}(z) - nj_n(z) \tag{168}$$

$$[zh_n(z)^{(1)}]' = zh_{n-1}(z)^{(1)} - nh_n(z)^{(1)} \tag{169}$$

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Verifying FEM correctness

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1 Introduction

From our formalism, we know that the FEM weak form is compactly represented as

$$\phi(\vec{T},\vec{E}) = b(\vec{T},\vec{E}_{inc}) \tag{1}$$

Here,
$\vec{E}$ is the unknown quantity: the total electric field as a function of space.
$\vec{T}$ is a known testing function (linear polynomial form)
$\vec{E}_{inc}$ is a known incident field function (plane wave)
ϕ and b are known operators.

In the Galerkin method, we translate the weak form to $\mathbf{Ax} = \mathbf{b}$ where $\mathbf{A}_{ij} = \phi(\vec{T}_i,\vec{T}_j)$ and $\mathbf{b}_i = b(\vec{T}_i)$

What do we want to do? Verify the correctness of the FEM code. The heart of FEM is coding up analytically obtained integrals for $\mathbf{A}_{ij}$. If the integrals are both correctly evaluated and correctly coded, a **manufactured vector field** $\vec{U}$ must numerically match the electric field profile generated using FEM in conjunction with $\vec{U}$.

1. Choose a suitable functional form $\vec{U}$
2. Compute $\widetilde{b}(\vec{T}) := \phi(\vec{T}_1,\vec{U})$ perfectly by hand and/or MATLAB. So $\widetilde{b}(\vec{T}_1)$ is now a known scalar value.

   Note that an optimal choice of $\vec{U}$ would be based on minimizing $|\widetilde{b}[\vec{U}] - b|$ subject to constraints on $\vec{U}$ in a suitable polynomial vector space. But I don't think it is necessary to indulge in that.
3. With the same $\vec{U}$, compute $\widetilde{b}(\vec{T}_2),\widetilde{b}(\vec{T}_3)\ldots\widetilde{b}(\vec{T}_N)$ for each global edge basis function in the computational domain. We would hence have the vector $\widetilde{\mathbf{b}}$
4. Use our FEM code to solve for $\mathbf{x}$ in $\mathbf{Ax} = \widetilde{\mathbf{b}}$
5. The correctness of evaluation and coding of FEM matrix $\mathbf{A}$ is confirmed if we observe a numerical match between $(x_1\vec{T}_1 + x_2\vec{T}_2\ldots x_N\vec{T}_N)$ and $\vec{U}$ when plotted on various slices of the computational domain.

Note that this procedure doesn't verify the evaluation or coding of the incident field vector $\mathbf{b}$.

The numerical match is expected to be best when $\vec{U}$ has a linear polynomial form, since the vector basis functions $\vec{T}$ in our case have a linear polynomial form in single tetrahedral elements and zero outside. Another consideration is that the electric field better be non-conservative ($\vec{U} \neq -\nabla V$), as expected of time-dependent fields.

We choose

$$\vec{U} = z\hat{x} + x\hat{y} + y\hat{z} \tag{2}$$

2 Weak form based approach

We want to evaluate

$$\tilde{b}(\vec{T}) = \phi(\vec{T},\vec{U}) \tag{3}$$

where

$$\phi(\vec{T},\vec{U}) = \int_\Omega \Big[(\nabla\times\vec{T})\cdot(\nabla\times\vec{U}) - k_0^2\epsilon_r\vec{T}\cdot\vec{U}\Big]\,dV + jk_0\sqrt{\epsilon_r}\oint_\Gamma \Big[\vec{T}\cdot\vec{U} - (\vec{T}\cdot\hat{n})(\vec{U}\cdot\hat{n})\Big]\,dS \tag{4}$$

with $\vec{U} = (z,x,y)$ as the manufactured solution.

Splitting it into 4 terms, we get

$$\tilde{b}(\vec{T}_k) = P_k - Q_k + R_k - S_k \tag{5}$$

Subscript k is used to denote local edge index.

2.1 P

$$P_k = \int_\Omega \Big[(\nabla\times\vec{T}_k)\cdot(\nabla\times\vec{U})\Big]\,dV \tag{6}$$

We know that

$$\nabla\times\vec{T}_k = \frac{l_k}{18V_e^2}\Big[(c_{k_1}d_{k_2} - c_{k_2}d_{k_1}),(d_{k_1}b_{k_2} - d_{k_2}b_{k_1}),(b_{k_1}c_{k_2} - b_{k_2}c_{k_1})\Big] \tag{7}$$

where l_k is the length of local edge k and V_e is the volume of the tetrahedron. The local edge k is joined by local nodes k_1 and k_2. And as we defined and used earlier, $\vec{T}_k = l_k(L_{k_1}\nabla L_{k_2} - L_{k_2}\nabla L_{k_1})$

Using $\nabla\times\vec{U} = (1,1,1)$,

$$\boxed{P_k = \frac{l_k}{18V_e}\Big[(c_{k_1}d_{k_2} - c_{k_2}d_{k_1}) + (d_{k_1}b_{k_2} - d_{k_2}b_{k_1}) + (b_{k_1}c_{k_2} - b_{k_2}c_{k_1})\Big]} \tag{8}$$

2.2 Q

$$Q_k = k_0^2\epsilon_r\int_\Omega \vec{T}_k\cdot\vec{U}dV \tag{9}$$

Note that

$$\vec{T}_k\cdot\vec{U} = l_k\Big[L_{k_1}(\nabla L_{k_2}\cdot\vec{U}) - L_{k_2}(\nabla L_{k_1}\cdot\vec{U})\Big] \tag{10}$$

Hence

$$\begin{aligned}\vec{T}_k\cdot\vec{U} &= \frac{l_k}{36V_e^2}\Big[(a_{k_1} + b_{k_1}x + c_{k_1}y + d_{k_1}z)(b_{k_2}z + c_{k_2}x + d_{k_2}y) - (a_{k_2} + b_{k_2}x + c_{k_2}y + d_{k_2}z)(b_{k_1}z + c_{k_1}x + d_{k_1}y)\Big]\\ &= \frac{l_k}{36V_e^2}\Big[\text{Linear terms} + \text{Quadratic terms}\Big]\end{aligned}$$

Linear terms:

$$[a_{k_1}b_{k_2} - a_{k_2}b_{k_1}]z + [a_{k_1}c_{k_2} - a_{k_2}c_{k_1}]x + [a_{k_1}d_{k_2} - a_{k_2}d_{k_1}]y \tag{11}$$

Quadratic terms:

$$\begin{aligned}&[b_{k_1}c_{k_2} - b_{k_2}c_{k_1}]x^2 + [c_{k_1}d_{k_2} - c_{k_2}d_{k_1}]y^2 + [d_{k_1}b_{k_2} - d_{k_2}b_{k_1}]z^2\\ &+[b_{k_1}d_{k_2} - b_{k_2}d_{k_1}]xy + [c_{k_1}b_{k_2} - c_{k_2}b_{k_1}]yz + [d_{k_1}c_{k_2} - d_{k_2}c_{k_1}]zx\end{aligned}$$

We shift to linear algebraic notation to simplify analysis. Let us represent the linear terms as $\alpha^T r$ and the quadratic terms as $r^T Ar$, defining $r = (x,y,z)$ as column vector. Hence

$$\vec{T}_k\cdot\vec{U} = \frac{l_k}{36V_e^2}\Big(\alpha^T r + r^T Ar\Big) \tag{12}$$

Where

$$\boxed{\alpha = \begin{bmatrix}(a_{k_1}c_{k_2} - a_{k_2}c_{k_1})\\(a_{k_1}d_{k_2} - a_{k_2}d_{k_1})\\(a_{k_1}b_{k_2} - a_{k_2}b_{k_1})\end{bmatrix} \quad \& \quad A = \begin{bmatrix}(b_{k_1}c_{k_2} - b_{k_2}c_{k_1}) & A_{12} & A_{13}\\ A_{21} & (c_{k_1}d_{k_2} - c_{k_2}d_{k_1}) & A_{23}\\ A_{31} & A_{32} & (d_{k_1}b_{k_2} - d_{k_2}b_{k_1})\end{bmatrix}} \tag{13}$$

There is freedom in the choice of off-diagonal entries of A subject to

$$\boxed{\begin{aligned} A_{12} + A_{21} &= (b_{k_1} d_{k_2} - b_{k_2} d_{k_1}) \\ A_{13} + A_{31} &= (c_{k_1} b_{k_2} - c_{k_2} b_{k_1}) \\ A_{23} + A_{32} &= (d_{k_1} c_{k_2} - d_{k_2} c_{k_1}) \end{aligned}}$$

Next, we transform the domain of integration from the tetrahedron $\texttt{conv}\{r_1, r_2, r_3, r_4\}$ in xyz space to the unit tetrahedron in uvw space [$\underline{u} = (u, v, w)$ as column vector] using a linear transformation

$$r = r_1 + J\underline{u} \tag{14}$$

The Jacobian matrix

$$\boxed{J = \begin{bmatrix} (r_2 - r_1) & (r_3 - r_1) & (r_4 - r_1) \end{bmatrix}} \tag{15}$$

Hence, we find that Equation (12) transforms as

$$\alpha^T r + r^T A r = \left[\alpha^T r_1 + r_1^T A r_1\right] + \left[\alpha^T + r_1^T (A + A^T)\right] J\underline{u} + \underline{u}^T J^T A J \underline{u} \tag{16}$$

And an arbitrary volume element transforms as $d^3 r = |J|\ d^3 u$. Also, note that over the unit tetrahedron,

$$\int u^p v^q w^r d^3 u = \frac{p!q!r!}{(p + q + r + 3)!} \tag{17}$$

Using this result, note that the following identities are true:

- $\int d^3 u = \frac{1}{6}$
- $\int c^T \underline{u}\ d^3 u = \frac{1}{24} c^T \mathbb{1}$
- $\int \underline{u}^T M \underline{u}\ d^3 u = \frac{1}{120} \left[\mathbb{1}^T M \mathbb{1} + \mathrm{Tr}(M)\right]$

where $\mathbb{1}$ is the column vector $(1, 1, 1)$ and Tr represents the trace operator. Using these results in conjunction with the transformed quadratic form (Equation 16), we finally have

$$\boxed{Q_k = \frac{|J|\ k_0^2 \epsilon_r\ l_k}{36 V_e^2} \left[\frac{1}{6}\left[\alpha^T r_1 + r_1^T A r_1\right] + \frac{1}{24}\left[\alpha^T + r_1^T (A + A^T)\right] J\mathbb{1} + \frac{1}{120}\left[\mathbb{1}^T J^T A J \mathbb{1} + \mathrm{Tr}(J^T A J)\right]\right]} \tag{18}$$

2.3 R

$$R_k = j k_0 \sqrt{\epsilon_r} \oint_\Gamma \vec{T}_k \cdot \vec{U} dS \tag{19}$$

From the previous section, we know

$$\vec{T}_k \cdot \vec{U} = \frac{l_k}{36 V_e^2} \left(\alpha^T r + r^T A r\right) \tag{20}$$

with α and A being defined in the same way as equation 13. Since $\vec{T}_k$ is a local basis function at a surface element, the domain of integration reduces to an exposed triangle $\Delta = \texttt{conv}\{r_1, r_2, r_3\}$. We now transform the domain of integration from the exposed triangle to a unit right triangle in a transformed space using the linear transformation

$$\vec{r} = \vec{r}_1 + \beta \vec{u} + \gamma \vec{v} \tag{21}$$

where β and γ are scalar variables whose range is the unit triangle in the $\beta - \gamma$ space, with

$$\boxed{\begin{aligned} \vec{u} &= \vec{r}_2 - \vec{r}_1 \\ \vec{v} &= \vec{r}_3 - \vec{r}_1 \end{aligned}}$$

Hence, spacial integrals transform as

$$\int f(r) dS = 2\ \mathrm{Area}(\Delta) \int f(r_1 + \beta u + \gamma v) d\beta d\gamma \tag{22}$$

In this simpler domain, polynomial terms integrate to simple closed form expressions

$$\int \beta^{c_1}\gamma^{c_2} d\beta d\gamma = \frac{c_1!c_2!}{(c_1+c_2+2)!} \tag{23}$$

In particular, (Let's call $d\beta d\gamma$ as dA)

- $\int dA = \frac{1}{2}$
- $\int \beta dA = \int \gamma dA = \frac{1}{6}$
- $\int \beta^2 dA = \int \gamma^2 dA = \frac{1}{12}$
- $\int \beta\gamma dA = \frac{1}{24}$

In our case, the integrand transforms as

$$\alpha^T r + r^T A r = \alpha^T(r_1+\beta u+\gamma v) + (r_1+\beta u+\gamma v)^T A(r_1+\beta u+\gamma v) \tag{24}$$

Expanding this, and using the results we know for polynomial terms, we have

$$\boxed{\begin{aligned} R_k = jk_0\sqrt{\epsilon_r}\ \text{Area}(\Delta)\frac{l_k}{18V_e^2}\Bigg[&\frac{1}{2}\left[\alpha^T r_1 + r_1^T A r_1\right] + \frac{1}{6}\left(r_1^T(A+A^T)+\alpha^T\right)(u+v) \\ &+\frac{1}{12}\left[u^T A u + v^T A v + 0.5u^T(A+A^T)v\right]\Bigg] \end{aligned}} \tag{25}$$

2.4 S

$$S_k = jk_0\sqrt{\epsilon_r}\oint_\Gamma (\vec{T}_k\cdot\hat{n})(\vec{U}\cdot\hat{n})dS \tag{26}$$

Here the normal vector $\hat{n}$ at surface elements is available to us through a C++ function, $\vec{U}$ is the manufactured solution, $\vec{T}_k$ is a local basis function at a surface element, and other symbols have their usual meanings.

$$\hat{n} = (n_x, n_y, n_z) \tag{27}$$

$$\vec{U} = (z, x, y) \tag{28}$$

Hence

$$\vec{U}\cdot\hat{n} = zn_x + xn_y + yn_z = \widetilde{n}^T r \tag{29}$$

where $\widetilde{n}$ is a permutation of $\hat{n}$ defined as

$$\boxed{\widetilde{n} = \begin{pmatrix} n_y \\ n_z \\ n_x \end{pmatrix}} \tag{30}$$

From our formalism, we know that

$$\vec{T}_k\cdot\hat{n} = \frac{l_k}{36V_e^2}\Big[(a_{k_1}\Psi_{k_2}-a_{k_2}\Psi_{k_1}) + (b_{k_1}\Psi_{k_2}-b_{k_2}\Psi_{k_1})x + (c_{k_1}\Psi_{k_2}-c_{k_2}\Psi_{k_1})y + (d_{k_1}\Psi_{k_2}-d_{k_2}\Psi_{k_1})z\Big] \tag{31}$$

Where Ψ_k is defined as

$$\Psi_k = b_k n_x + c_k n_y + d_k n_z \tag{32}$$

A linear algebraic form of Equation (31) would be

$$\vec{T}_k\cdot\hat{n} = \frac{l_k}{36V_e^2}\left(G + h^T r\right) \tag{33}$$

with

$$\boxed{h = \begin{pmatrix} (b_{k_1}\Psi_{k_2}-b_{k_2}\Psi_{k_1}) \\ (c_{k_1}\Psi_{k_2}-c_{k_2}\Psi_{k_1}) \\ (d_{k_1}\Psi_{k_2}-d_{k_2}\Psi_{k_1}) \end{pmatrix} \qquad \& \qquad G = (a_{k_1}\Psi_{k_2}-a_{k_2}\Psi_{k_1})} \tag{34}$$

Now Equation (29) and Equation (31) are multiplied, and we define use a matrix intermediate variable

$$\boxed{M = h\ \widetilde{n}^T} \tag{35}$$

and then perform the same linear transformation as in the previous section (for R) and evaluate the integral to be

$$\boxed{\begin{aligned} S_k = jk_0\sqrt{\epsilon_r}\ \text{Area}(\Delta)\frac{l_k}{18V_e^2}\Bigg[\frac{1}{2}\left[G\widetilde{n}^T r_1 + r_1^T M r_1\right] + \frac{1}{6}\left(r_1^T(M + M^T) + G\widetilde{n}^T\right)(u+v) \\ + \frac{1}{12}\left[u^T M u + v^T M v + 0.5u^T(M + M^T)v\right]\Bigg] \end{aligned}} \tag{36}$$