Inverse electromagnetics scattering problem

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Computation of electromagnetic caracteristics of body can be performed with integral formulation equation. With finite element method on surface of body we obtain descrete formulation of problem. Firstly, I will present variational approach using the reaction concept of Rumsey and combining electric integral equation (EFIE) and magnetic integral equation (MFIE). Beside this, we have to take into consideration Huyghens principle that is applied at interfaces between every homogenous volume. After using code that is devoloped in Turbie and that solves Integral equation using 2-D finite element method we will get information about scattered field. Having the data about value of field and first derivative we can do Hermite interpolation. Interpolation will be done if for 3 values of dielectric constant for which we have value of scattered field and first derivative. Polynomial is of degree 5. After reading value for which we want to compute dielectrical constant we can find eigenvalues of corresponding companion matrix using numerical method (QR method). Fortran code is checking whether eigenvalues are real and in range [ε_{min} , ε_{max}]. Moreover, Matlab code that is written gives us graphical presentation of Hermite interpolation and how it coincide with results of simulation code that is done in Turbie.

1 Electromagnetics

Time Domain in comparison with Frequency Domain

For equations that are inherently nonlinear we can't use Fourier transform methods. For many applications the electromagnetic equations are linear. So we have possibility to solve the electromagnetic equations in the frequency domain other than the time domain. The frequency-domain equations are obtained by Fourier transforming the electromagnetic equations in time. The advantages of solving the electromagnetic equations in the frequency domain is the fact that they don't depend on time, and hence the resultant equations are simpler, so for example derivative with respect to time is equivalent with multiplication with $-i\omega$ in frequency domain. Another advantage is that each frequency component solution can be solved independently, they can be solved parallely with no intersection between frequences. Time domain solutions can be obtained after superposition of solution for different frequencies.

Differential Equation versus Integral Equation

We are solving the equations in their differential forms in the case when we have nonlinear problem. If a problem is linear, the principle of linear superposition enables us to first derive the point source response of the differential equation, so called Green's function that is the fundamental solution of the differential equation. If we know the Green's function, we can derive an integral equation whose solution solves the problem. For a wave equation in time domain:

$$\nabla^2 \phi(r,t) - \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \phi(r,t) = s(r,t)$$

If wave function is proportional to e^{-iwt} the equation becomes the Helmholtz equation :

$$\nabla^2 \phi(r,w) - k^2 \frac{\partial^2}{\partial t^2} \phi(r,w) = s(r,w)$$

where $k{=}w/v$. The Green's function is the solution when the right-hand side is replaced by a point source :

$$\nabla^2 g(r, r') + k^2 g(r, r') = -\delta(r - r')$$

If we assume linearity by the principle of superposition we can express Green's function as:

$$\phi(r,w) = -\int_{V} g(r,r')s(r',w)dr'$$

We can use these integral equation to express scattering where $\phi(r, w)$ is incident field and Green's function for free space is expressed as:

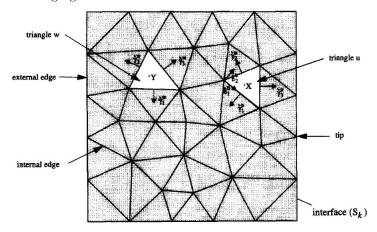
$$g(r, r') = \frac{e^{ik|r-r'|}}{4\pi|r-r'|}$$

where k is wave number such that $k^2 = \varpi^2 \varepsilon_r \mu_r$. Solving this equation implies to find source. Advantage of solving equation of this type is that in our case it is the fact that source is spread on 2-D manifold or surface. In comparison with differential equation, this integral type has less unknowns. One more advantage of integral equation is the fact that Green's function is exact propagator of field. There is no grid dispersion error like in numerical differential equations solvers where the field is propagated over numerical grid. Grid dispersion error is causing error in phase velocity, and it's serious problem.

Disadvantage of integral equations are their solvers that are much more complicated for implemetation in comparison with numerical differential equations solvers. On the other hand, numerical differential equation solvers are easier to implement compared to integral equation solvers. The differential equation solver deals with sparse matrix system so we can reduce storage requirements (O(N) storage for problem with N unknown), but the matrix system associated with integral equation is usually a dense matrix system requiring $O(N^2)$ storage and more than $O(N^2)$ central processing unit (CPU) time to solve. Previously, only dense matrix systems with tens of thousands of unknowns can be solved, but now, dense matrix systems with tens of millions of unknowns can be solved .

We will observe 3D structure that is divided into N homogenous domains with different dielectric carcterisites ε_r , μ_r , in each of them classical Maxwell's equations are valid.

In following figure we can see mash on the surface:



Regarding boundary conditions, between two domains Ω_k and Ω_l , for \vec{E} and \vec{H} is valid following :

$$\vec{n_k} \times \vec{E_k} + \vec{n_l} \times \vec{E_l} = 0 = \vec{m_k} + \vec{m_l}$$
$$\vec{n_k} \times \vec{H_k} + \vec{n_l} \times \vec{H_l} = 0 = \vec{j_k} + \vec{j_l}$$

Using Green's representation formula for each domain Ω_k that is bounded by S_k we can obtain integral equations that gives us information about electromagnetic field and they express in electromagnetics so called Huyghens principle. This principle means that wave in each point is in fact the center of disturbance and the source of a new waves; and that wave as a whole is superposition of all the secondary waves arising from points in the medium already traversed.

$$\vec{E_k}(x) = \vec{E_k}^i + i\omega\mu \oint_{(S_k)} G(x, y) \vec{j_k}(y) ds(y) - \frac{1}{i\omega\epsilon} \oint_{(S_k)} grad_x G(x, y) div_{S_k} \vec{j_k}(y) ds(y) - rot \oint_{(S_k)} G(x, y) \vec{m_k}(y) ds(y) ds$$

$$\vec{H_k}(x) = \vec{H_k^i} + i\omega\epsilon \oint_{(S_k)} G(x, y) \vec{m_k}(y) ds(y) - \frac{1}{i\omega\mu} \oint_{(S_k)} grad_x G(x, y) div_{Sk} \vec{m_k}(y) ds(y) - rot \oint_{(S_k)} G(x, y) \vec{j_k}(y) ds(y) ds($$

where $G(x,y) = \frac{e^{ikR}}{4\pi R}$ is green function for open space, R = |x - y|, x is observation point in corresponding domain, y is source point on surface,

 $div_{Sk}\vec{j} = [\nabla - (\vec{n_k}\vec{\nabla})\vec{n_k}]\vec{j}$, $\vec{E_k}^i(x)$ is incident electric field associated with Ω_k and $\vec{H_k}^i$ is magnetic incident field.

So we conclude that integral equations are in function of j_k and m_k in the surface of each homogenous domain Ω_k .

Third term in first equation can be expressed over electric charge :

$$\frac{1}{i\omega\epsilon} \oint_{(S_k)} grad_x G(x,y) div_{Sk} \vec{j_k}(y) ds(y) = \frac{1}{\varepsilon} grad \oint_{(S_k)} G(x,y) \rho(y) ds(y) ds(y$$

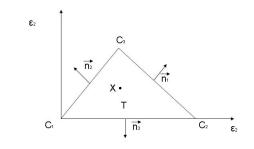
Finally, introducing test vector \vec{j}^t and \vec{m}^t and combining it with boundary condition and Green representation we will obtain variational formulation:

$$\sum_{l=1}^{N} \mu_{rl} Q_{Sl}(S_t, j_l, j_l^t) + \frac{k_l^2}{\mu_{rl}} Q_{sl}(S_t, m_l, m_l^t) - P_{sl}(S_t, j_l, m_l^t) - P_{sl}(S_t, m_l, j_l^t) = -\sum_{l=1}^{N} \oint_{Sl} (E_l^i(x) j_l^t - H_l^i(x) m_l^t) ds(x) + \sum_{l=1}^{N} \frac{1}{2} \int_{Sl} \frac{1}{2} \left(\frac{1}{2} \int_{Sl} \frac{1}$$

where P_{sl} and Q_{sl} are defined as :

$$\begin{aligned} Q_{Sl}(S_t, j_l, j_l^t) &= \oint_{S^t} \oint_{S^l} G(k, x, y) (j(y)j^t(x) - \frac{1}{k_l^2} div_S j(y) div_{S^t} j^t(x)) ds(x) ds^t(y) \\ P_{Sl}(S_t, j_t, m_l^t) &= \oint_{S^t} \oint_{S^l} [grad(G(k, x, y) \times j(y))] p^t(x) ds(y) ds^t(x) \end{aligned}$$

Using 2-D finite element method we will obtain discretization of the suface of structure (triangular type with 6 degrees of freedom by triangle). Following equation is transformed into system of discrete equation where electric and magnetic current densities are unknown. They devolop base associated with triangles.



 $x = C_1 + \zeta_1 \vec{\varepsilon_1} + \zeta_2 \vec{\varepsilon_2}$

$$\vec{j(x)} = \alpha_1 \vec{\varepsilon_1} + \alpha_2 \vec{\varepsilon_2} + \beta \vec{C_1 x}$$
$$\vec{j(x)} = \frac{1}{area(T)} (J_1^T \vec{C_1 x} + J_2^T \vec{C_2 x} + J_3^T \vec{C_3 x})$$
where

where

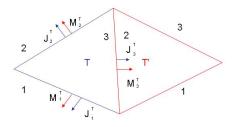
$$J_w^T = \oint_{\substack{ \overrightarrow{C_w C_v}}} \vec{n_w} \bullet j(\vec{x}) ds$$

Bilinear form is tranformed into descrete one :

$$\sum_{l=1}^{N}\sum_{u=1}^{NE_{1}}\sum_{w=1}^{NE_{1}}\mu_{rl}A_{l}^{uw}(\overrightarrow{j_{l}},\overrightarrow{j_{l}}) + \frac{k_{l}^{2}}{\mu_{rl}}A_{l}^{uw}(\overrightarrow{p_{l}},\overrightarrow{p_{l}}) - B_{l}^{uw}(\overrightarrow{j_{l}},\overrightarrow{j_{l}}) - B_{l}^{uw}(\overrightarrow{p_{l}},\overrightarrow{p_{l}}) = \sum_{l=1}^{N}\sum_{w=1}^{NE_{1}}C_{l}^{w}(\overrightarrow{E_{l}},\overrightarrow{H_{l}},\overrightarrow{j_{l}},\overrightarrow{p_{l}}) - B_{l}^{uw}(\overrightarrow{j_{l}},\overrightarrow{j_{l}}) - B_{l}^{uw}(\overrightarrow{p_{l}},\overrightarrow{p_{l}}) - B_{l}^{uw}($$

Summation is done on N domains and on NE_1 triangles of mash of the body surface. Matrix formulation of previous equation is Ax=C, where A is matrix of coupling between different triangles that is function of reaction elements A^{uw} and B^{uw} . X is vector with unknown current densities. C is vector that is composed of elements C_l^w that desribe effect of test currents on incident electromagnetic field.

Expression of currents on triangles



Currents of the triangle T can be expressed as it is written:

$$\vec{j^T} = \vec{j_1^T} \cdot J_1^T + \vec{j_2^T} \cdot J_2^T + \vec{j_3^T} \cdot J_3^T$$

$$\vec{m^T} = M_1^T \cdot \vec{m_1^T} + M_2^T \cdot \vec{m_2^T} + M_3^T \cdot \vec{m_3^T}$$

so for the two neighbouring triangles we can write:

$$-J_2^{T'} = J_3^T = J_k$$

and conclude that we have 6 degrees of freedom.

2 Hermite interpolation

In numerical mathematics Hermit interpolation method is used along with Newton divided differences. We can take advantage of having data about derivative in some point.

Hermite(Osculating) polynomials are generalization of both the Taylor and Langrangian polynomials. If we have given n+1 points $x_0, x_1, ..., x_n$ and nonnegative integers $m_0, ...$ Hermite polynomial approximating a function f is polynomial of at least degree of m_i at point x_i where f belongs to $C^m(a, b)$ and m = max{ $m_0, ..., m_n$ } and x_i belongs to [a,b] for every i = 0, ... n.

The degree of this osculating polynomial will be at most :

$$M = \sum_{i} m_i + n.$$

The number of conditions to be satisfied is $\sum_{i} m_i + (n+1)$ and a polynomial of degree M has M+1 coefficients that has to satisfy these conditions.

By definition, if we have n+1 distinct numbers in range [a,b] and m_i are nonnegative integers associated with x_i , so for each i = 0, ..., n.

If $\mathbf{m} = \max_{0 \le i \le n} m_i$ and $\mathbf{f} \in C^m[a, b]$

so Hermite polynomial approximating f is the polynomial P of least degree m such that $\frac{d^k P(x_i)}{dx^k} = \frac{d^k f(x_i)}{dx^k}$ for each i =0, 1, ..., n and k=0,1, ..., m_i .

We can notice that in case n=0 Hermite polynomial that approximates f is simply $m_o - th$ Taylor polynomial in point x_o . In case when $m_i = 0$ for i =0, 1, ..., n, the Hermite polynomial is the n-th Langrange polynomial interpolating f on $x_0, x_1, ..., x_n$. If $m_i = 1$ for each i = 0, ..., n we have a class of so called Hermite polynomials. For function f these polynomials agree with f at $x_0, x_1, ..., x_n$, additionally since their first derivatives are equal they have the same shape s the function f.

If the function f belongs to $C^1[a, b]$ and x_0, x_1, \dots, x_n that are in range [a,b] are distinct, tha unique polynomial of least degree matching with f and f' at x_0, x_1, \dots, x_n is the polynomial of degree at most M=2n+1 given as :

$$H_{2n+1}(x) = \sum_{j} f(x_j) H_{n,j}(x) + \sum_{j} f'(x_j) \hat{H}_{n,j}(x)$$

where :

$$H_{n,j}(x) = [1 - 2(x - x_j)L'_{n,j}(x_j)]L^2_{n,j}(x)$$

 and

$$\stackrel{\wedge}{H}_{n,j}(x) = (x - x_j)L_{n,j}^2(x)$$

here $L_{n,j}(x)$ denotes Langrange coefficient polynomial of degree n that si defined by formula :

$$L_{n,k}(x) = \frac{(x-x_0)\dots(x-x_{k-1})(x-x_{k+1})\dots(x-x_n)}{(x_k-x_0)\dots(x_k-x_{k-1})(x_k-x_{k+1})\dots(x_k-x_n)}$$

For function f that belongs to $C^{2n+2}[a, b]$, then $f(\mathbf{x}) = H_{2n+1}(x) + \frac{(x-x_0)^2 \dots (x-x_n)^2}{(2n+2)!} f^{(2n+2)}(\xi)$ with some ξ such that $a < \xi < b$.

PROOF:

Regarding $L_{n,j}(x)$ we know that $L_{n,j}(x)$ is equal to zero if $i \neq j$. Otherwise is equal to 1. So if we consider $i \neq j$ we have following relations:

 $H_{n,j}(x_i) = 0$ and $\stackrel{\wedge}{H}_{n,j}(x_i) = 0$

also we can conclude that :

$$H_{n,i}(x) = [1 - 2(x_i - x_i)L'_{n,i}(x_i)] \cdot 1 = 1$$

and

$$\hat{H}_{n,i}(x_i) = (x_i - x_i) \cdot 1^2 = 0$$

Thus we obtain that H_{2n+1} coincide with f at points x_0, x_1, \ldots, x_n :

$$\begin{aligned} H_{2n+1}(x_i) &= \sum_{j \neq i} f(x_j) \cdot 0 + f(x_i) \cdot 1 + \sum_j f'(x_j) \cdot 0 = f(x_i) \\ \text{Since } L_{n,j}(x) \text{ is a factor of } H'_{n,j}(x) \text{ , for } i \neq j \text{ both of them are equal to zero.} \\ \text{In the case when } i &= j : \\ H'_{n,i}(x_i) &= 2 \cdot [1 - 2(x_i - x_i)L'_{n,i}(x_i)]L_{n,i}(x_i) \cdot L'_{n,i}(x_i) - 2L^2_{n,i}(x_i) \cdot L'_{n,i}(x_i) = 0 \\ \text{So for all values of i and } j : H'_{n,i}(x_i) = 0 \\ \stackrel{\wedge}{H}'_{n,j}(x_i) &= 2(x_i - x_j)L_{n,j}(x_i)L'_{n,j}(x_i) + L^2_{n,j}(x_i) \end{aligned}$$

This derivative is 0 when $i \neq j$, and $\stackrel{\wedge}{H}'_{n,i}(x_i) = 1$ so we can compute that $H'_{2n+1}(x_i)$ coincide with f' at x_0, x_1, \ldots, x_n .

$$H'_{2n+1}(x_i) = \sum_{j} f(x_j) \cdot 0 + \sum_{i \neq j} f'(x_j) \cdot 0 + f'(x_i) \cdot 1 = f'(x_i)$$

Evaluation of Langrange polynomials and derivatives is difficult even for small n. Alterntive method for determination Hermitian polynomials is based on Newton interpolary divided difference formula.

Newton divided differences

For a function interpolated at points x_0, x_1, \ldots, x_n , the interpolation polynomial for a given set of points is in Newton form. Coefficients of the polynomial are calculated using divided differences as it is shown in following table.

So we can introduce zero-th dividived difference in $x_i - th$ point as $f(x_i) = f[x_i]$.

First divided difference with respect to points x_i and x_{i+1} will be : $f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}$.

To summarize k-th divided difference with respect to $x_i, x_{i+1}, \dots, x_{i+k}$ will be :

x	f(x)	First divided differnces	Second divided differences	Third divided differences	
x_0	$f[x_0]$				
		$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0}$			
x_1	$f[x_1]$		$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$		
		$f[x_1, x_2] = \frac{f[x_2] - f[x_1]}{x_2 - x_1}$		$f[x_0, x_1, x_2, x_3] = \frac{f[x_1, x_2, x_3] - f[x_0, x_1, x_2]}{x_3 - x_0}$	
x_2	$f[x_2]$		$f[x_1, x_2, x_3] = \frac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1}$		
		$f[x_2, x_3] = \frac{f[x_3] - f[x_2]}{x_3 - x_2}$		$f[x_{1,x_{2},x_{3,x_{4}}] = \frac{f[x_{2,x_{3},x_{4}}] - f[x_{1,x_{2},x_{3}}]}{x_{4} - x_{1}}$	
x_3	$f[x_3]$		$f[x_2, x_3, x_4] = \frac{f[x_3, x_4] - f[x_2, x_3]}{x_4 - x_2}$		
		$f[x_3, x_4] = \frac{f[x_4] - f[x_3]}{x_4 - x_3}$		$f[x_{0,}x_{1}, x_{2}, x_{3}] = \frac{f[x_{3,}x_{4}, x_{5}] - f[x_{2,}x_{3}, x_{4}]}{x_{5} - x_{2}}$	
x_4	$f[x_4]$		$f[x_3, x_4, x_5] = \frac{f[x_4, x_5] - f[x_3, x_4]}{x_5 - x_3}$		
		$f[x_4, x_5] = \frac{f[x_5] - f[x_4]}{x_5 - x_4}$			
x_5	$f[x_5]$				

$$f[x_{i,x_{i+1},\dots,x_{i+k}] = \frac{f[x_{i+1},\dots,x_{i+k}] - f[x_i,x_{i+1}\dots,x_{i+k-1}]}{x_{i+k} - x_i}$$

For the Langrange polynomial $P_n(x) = f[x_0] + \sum_{k=1}^n f[x_0, x_1, ..., x_k](x - x_0)(x - x_1)....(x - x_{k-1})$ and for the given points $x_0, x_1, ..., x_n$, we will assume that we have values of f and f' in all of these points and we will define following sequence $z_0, z_1, ..., z_{2n}, z_{2n+1}$ such that for every i that belongs to (0,n):

$$z_{2i} = z_{2i+1} = x_i$$

First divided differences we can express over values $f'(x_i)$:

$$f[z_{2i}, z_{2i+1}] = f'[z_{2i+1}] = f'(x_i)$$

Example:

Hermite polynomial for points x_0, x_1, x_2 is : $H_5 = f[z_0] + \sum_{k=1}^{2n+1} f[z_0, ..., z_k](x-z_0)(x-z_1)...(x-z_{k-1}).$ Here is the corresponding table:

z	f(z)	First divided differnces	Second divided differences					
$z_0 = x_0$	$f[z_0] = f[x_0]$							
		$f[z_0, z_1] = f'(x_0)$						
$z_1 = x_0$	$f[z_1] = f[x_0]$		$f[z_0, z_1, z_2] = \frac{f[z_1, z_2] - f[z_0, z_1]}{z_2 - z_0}$					
		$f[z_1, z_2] = \frac{f[z_2] - f[z_1]}{z_2 - z_1}$						
$z_2 = x_1$	$f[z_2] = f[x_1]$		$f[z_1, z_2, z_3] = \frac{f[z_2, z_3] - f[z_1, z_2]}{z_3 - z_1}$					
		$f[z_2, z_3] = f'(x_1)$						
$z_3 = x_1$	$f[z_3] = f[x_1]$		$f[z_2, z_3, z_4] = \frac{f[z_3, z_4] - f[z_2, z_3]}{z_4 - z_2}$					
		$f[z_3, z_4] = \frac{f[z_4] - f[z_3]}{z_4 - z_3}$						
$z_4 = x_2$	$f[z_4] = f[x_2]$		$f[z_3, z_4, z_5] = \frac{f[z_4, z_5] - f[z_3, z_4]}{z_5 - z_3}$					
		$f[z_4, z_5] = f'(x_2)$						
$z_5 = x_2$	$f[z_5] = f[x_2]$	11 1 . • •						

So polynomial that we will obtain is:

 $H(x) = Q_{0,0} + (x - x_0)Q_{11} + Q_{2,2}(x - x_0)^2 + Q_{3,3}(x - x_0)(x - x_1) + Q_{4,4}(x - x_0)^2(x - x_1)^2 + Q_{5,5}(x - x_2)(x - x_0)^2(x - x_1)^2$

When we have information about scattered field, we can do interpolation. It's enough to have coefficients of osculating polynomials we can obtain value of dielectric constant for some value of scattered field. Field is expressed as function of dielectric constant :

$$E(\varepsilon) = c_5\varepsilon^5 + c_4\varepsilon^4 + c_3\varepsilon^3 + c_2\varepsilon^2 + c_1\varepsilon + c_0$$

So if we know $E(\varepsilon)$ all we need to do is to modify coefficient c_0 and to find zeros of following polynomial:

$$c_5\varepsilon^5 + c_4\varepsilon^4 + c_3\varepsilon^3 + c_2\varepsilon^2 + c_1\varepsilon + c' = 0$$

where $c' = c_0 - E(\varepsilon)$.

Instead of finding zeros of previous polynomial we can look for eigenvalues of companion matrix :

($-\frac{c_4}{c_5}$	$-\frac{c_3}{c_5}$	$-\frac{c_2}{c_5}$	$-\frac{c_1}{c_5}$	$-rac{c'}{c_5}$
	1	0	0	0	0
$\mathbf{A} = $	0	1	0	0	0
	0	0	1	0	0
(0	0	0	1	0)

3 QR method for computing eigenvalues

QR decomposition of matrix A implies searching for matrix Q and R such that A = QR where R is uper triangular matrix and Q is unitary matrix $(Q \cdot Q^T = I)$.

We can conclude that if A has full column rank, then columns of Q form an orthonormal basis for ran(A). So this QR method is one way to compute an orthonormal basis for a set of vectors(in this case columns of matrix A). There are several ways to proceed computations like Householder, Givens rotations and fast Givens transformations. I was using Gram-Schmidt orthogonalization process (a numerically more stable variant called modified Gram-Schmidt).

Classical Gram-Schmidt

Gram-Shmidt implies orthogonalizing a set of vectors (in this case columns of matrix A) in an inner product Eucleadian space. Its used for QR decomposition of matrix A that can be presented as $A = Q_1 R_1$. If the column vectors are of a full column rank then application of Gram-Shmidt yields the QR decomposition. Fist we need to define projection of column a_i on vector q_i :

$$proj_{u_j}a_i = \frac{\langle a_i, u_j \rangle}{\langle u_j, u_j \rangle} u_j$$

if first step :

 $u_1 = a_1$ and $q_1 = \frac{u_1}{||u_1||}$

for the computation of k-th column of matrix **Q** we use formula :

$$u_k = a_k - \sum_{j=1}^{k-1} proj_{u_j} a_k$$

and column q_k :

$$q_k = \frac{u_k}{||u_k||}$$

Vectors $u_1, ..., u_n$ are orthogonal vectors and vectors $q_1, ..., q_n$ form an orthonormal set of vectors. These vectors are normalized and orthogonal and we call these process Gram-Schmidt orthonomalization. In order to obtain eigenvalues of matrix A, in each k-th step we first factorize matrix A :

$$A^k = Q * R$$

and then we compute new matrix A :

$$A^{k+1} = R * Q$$

After certain number of iteration we will have convergence. We can fix number of iteration or we can iterate until we achieve some accuracy.

Classical Gram Schmidt that is present doesn't have good numerical properties if we will use this method to calculate eignevalues, we will have loss of orthogonality. By checking product $Q * Q^t$ we will see that Classical method cannot work. We have to use modified Gram -Scmidt orthonormalization. Algorithm is following:

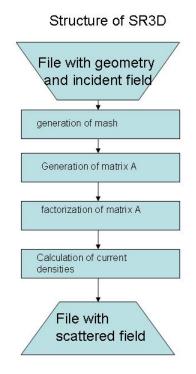
$$\begin{array}{l} {\rm do} \ k{=}1{,}5 \\ {\rm r}({\rm k}{,}{\rm k}){=}{\rm sqrt}({\rm dot_product}({\rm A}(1{:}5{,}{\rm k}){,}{\rm A}(1{:}5{,}{\rm k}))) \\ {\rm q}(1{:}5{,}\,{\rm k}) \,=\, {\rm A}(1{:}5{,}\,{\rm k}) \ / \ {\rm r}({\rm k}{,}{\rm k}); \end{array}$$

do j = k+1,5 r(k, j) = dot_product(q(1:5, k), A(1:5, j)); A(1:5, j) = A(1:5, j) - r(k, j) * q(1:5, k); end do end do

From the following algorithm we see that we this algorithm requires $2 * n^3$. If we compare this with Householder we conclude it is twice more efficient (since Householder requires $2n^3 - \frac{2n^3}{3}$ for the factorization and the same number of flops for geting first n columns of Q).

4 Short description of my program

My Fortran code reads data from file CHAMP.txt and calculates azimutal component of electromagnetic field. File CHAMP.txt contains information about scattered field that is calculated with respect to incident field, geompetry of body and coordinates of point where we are doing measurement. Computation is done with code SR3D.



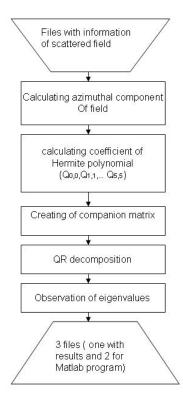
Program developed in Turbie is calculating scattered field with respect to incident field and geometry of the body. In my case it will be homogenous dielectric cube excited with dipole. At the first place is done mashing, then creation of matrix of coupling. After factorization of that matrix , current densities are computed. At the end this code computes scattered field.

With respect to value of field and its first derivative for 3 values of dielectrical constant interpolation is done. Degree of Hermite polynomial is 5. Small modifincations of program SR3D need to be done in order to obtain first derivative of scattered field. First we need to know derivative of incident field, besides this information this program needs data file with current densities, and geometry of body. Here unknown variable will be derivative of current densities.

When we obtain Hermite polynomial we transform it into standard form:

$$E(\varepsilon) = c_5\varepsilon^5 + c_4\varepsilon^4 + c_3\varepsilon^3 + c_2\varepsilon^2 + c_1\varepsilon + c_0$$

Then for some value of field we want to calculate dielectrical constant: we read that value and we modify coefficient c_0 . So our problem is to find zeros of that modified polynimal. We can use some method, like Newton Rapson, but if we start far from solution we will have divergence. Moreover, we can search for eigenvalues of companion matrix. I was using numerical method for computing eigenvalues so called QR method that is based on decomposition of matrix. There are several ways to do it but I was using Modified Gram-Schmidt.



Short description of my Matlab code

My Matlab code should give some graphical presentation of interpolation. Hermit polynomial is plotted along with values of field that are obtained with code SR3D.

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