MAS-Based Computer Simulation of 3D Frequency-Selective Surfaces

David Karkashadze(1), David Kakulia(1), Giorgi Ghvedashvili(1),
Kakhaber Tavzarashvili(2), Christian Hafner(2)

(1)Laboratory of Applied Electrodynamics at GPD, Tbilisi State University, Georgia
e-mail: davidkarkashadze@laetsu.org

(2)Laboratory for Electromagnetic Fields and Microwave Electronics,
Swiss Federal Institute of Technology, Zürich
e-mail: k.tavzarashvili@ifh.ee.ethz.ch,
christian.hafner@ifh.ee.ethz.ch
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The head of LAE is Prof. Revaz Zaridze and the head of Theoretical Department of LAE is Prof. David Karkashadze.

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The Head of LAE

Prof. David Karkashadze
The Head of Theoretical Department

Giorgi Ghvedashvili
Researcher staff member

David Kakulia
Researcher staff member

Giorgi Chelidze
Scientific worker

Gia Saparishvili
Researcher engineer

Levan Shoshiashvili
Engineer

Tamar Gogua
Laboratory assistant

Ph.D. Student members
Giorgi Kajaia
Ph. D. Student, Researcher
Dmitri Loskutov
Ph. D. Student, Researcher
Eresti Jakobia
Ph. D. Student, Researcher

Student members
Alexander Razmadze
M. S. (Computer Simulation)
Vaso Tabatadze
M. S. (General Physics)
Alex Bijanov
III year B. S. Student
Dimitry Mazmanov
III year B. S. Student
Nino Jejelava
II year B. S. Student
Liana Manukyan
II year B. S. Student
Outline

• Introduction
• MAS-MoM concepts for 2D and 3D periodic structures
• Model-Based Parameter Estimation (MBPE) technique
• Validation and Computer Simulation of 2D and 3D Periodic Structures
• MAS Geometry Editors and Visualization Tools
• Conclusion
Introduction: Scattering and Refraction From Periodic 3D structures

**Problem Formulation:**

**Scattering** and **Refraction** from Infinite, multilayered structure with double periodicity

**Incident Field** - either plane wave or superposition of several plane waves

Wide range of **Geometry** and **Material Properties**

**To be Investigated:**

the **Refraction** and **Transmission Coefficients** in wide frequency band

**Available software:**

Fast and accurate **MAS + MMP + FDTD** solvers

**Model-Based Parameter Estimation** technique (speed up frequency-dependence computations)

**Geometry Editors** and **Visualization Tools**

A.N. Grigorenko and all “Nanofabricated media with negative permeability at visible frequencies”, Vol 438|17 November 2005, Nature Letters
Biisotropic (4-parameter) mediums

Biisotropic properties of metamaterials are obtained by periodic inclusions of appropriate structural elements into isotropic materials

\[ \vec{D} = \varepsilon \vec{E} + i \alpha \vec{B}, \quad \vec{H} = i \beta \vec{E} + \frac{1}{\mu} \vec{B} \]

\( (\alpha = \beta \neq 0) \quad \text{Chiral,} \quad (\alpha = -\beta) \quad \text{Tellegen,} \)

\( (\alpha = \beta = 0) \quad \text{Magnetodielectrics,} \)

\( \alpha \text{ and } \beta - \text{chirality admintances} \)
Examples of Structural Elements

Left- or Right- handed elements, are responsible for chirality - their common effect in the media gives rise to biisotropic admittances.
General MAS code structure

For given constitutive relations
\[ \vec{D} = f_\varepsilon(\vec{E}, \vec{B}), \quad \vec{H} = f_\mu(\vec{E}, \vec{B}) \] : analytically derive wave equations, select potentials …

Fundamental and singular solutions of the wave equation

Where should singularities of the fundamental solutions (auxiliary sources) be placed?

Finding the best placement and type of the fundamental solutions, i.e., auxiliary sources (AS)

Numerical method to evaluate the amplitudes of the auxiliary sources

Method of collocation, method of moments (MOM), weighted residuals, and others

System of linear algebraic equations

Computation of the amplitudes of the AS
References

- Vekua I. About a metaharmonic functions. Georgia, 12(1943), 105-174.


Biisotropic (4-parameter) mediums

<table>
<thead>
<tr>
<th>Maxwell equations</th>
<th>Constitutive Relations</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. ( \text{rot} \vec{E} = i\omega \vec{B} ); II. ( \text{div} \vec{B} = 0 );</td>
<td>( \vec{D} = \varepsilon \vec{E} + i\alpha \vec{B} ), Isotropic magnetodielectrics when ( \alpha = \beta = 0 )</td>
</tr>
<tr>
<td>III. ( \text{rot} \vec{H} = -i\omega \vec{D} ); IV. ( \text{div} \vec{D} = 0 ).</td>
<td>( \vec{H} = i\beta \vec{E} + \frac{1}{\mu} \vec{B} ), Chiral medium when ( \alpha = \beta \neq 0 )</td>
</tr>
</tbody>
</table>

I. \( \text{Isotropic magnetodielectrics when } \alpha = \beta = 0 \)
II. \( \text{Chiral medium when } \alpha = \beta \neq 0 \)
III. \( \text{Tellegen medium when } \alpha = -\beta \neq 0 \)

\[ \vec{V}^2 \vec{U} + k^2 \vec{U} + \omega \mu (\alpha + \beta) \vec{V} \times \vec{U} = 0, \quad \vec{U} \text{ -- any field vectors} \]

<table>
<thead>
<tr>
<th>Material parameters</th>
<th>Wave impedances</th>
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</thead>
<tbody>
<tr>
<td>( \hat{\varepsilon} = \begin{pmatrix} \varepsilon^r &amp; 0 \ 0 &amp; \varepsilon^l \end{pmatrix}, \varepsilon^{r,l} = \frac{k^{r,l}}{\omega \eta^{r,l}}, ) ( \hat{\mu} = \begin{pmatrix} \mu^r &amp; 0 \ 0 &amp; \mu^l \end{pmatrix}, \mu^{r,l} = \frac{k^{r,l} \eta^{r,l}}{\omega} )</td>
<td>( \hat{\eta} = \begin{pmatrix} \eta^r \ \eta^l \end{pmatrix}, \eta^{r,l} = \eta_0 \cdot \left( \sqrt{\eta^2 + \frac{(\alpha + \beta)^2}{4}} \pm \frac{\alpha + \beta}{2} \right)^{-1} )</td>
</tr>
<tr>
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<td>( \eta_0 = \sqrt{\frac{\mu_0}{\varepsilon_0}}, \quad \eta = \sqrt{\frac{\mu_r}{\varepsilon_r}} )</td>
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</tbody>
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<tr>
<th>Wave number</th>
<th></th>
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<tbody>
<tr>
<td>( \hat{k} = \begin{pmatrix} k^r &amp; 0 \ 0 &amp; -k^l \end{pmatrix}, \quad k^{r,l} = k \cdot \eta \cdot \left( \sqrt{\eta^2 + \frac{(\alpha + \beta)^2}{4}} \pm \frac{\alpha + \beta}{2} \right), \quad k = k_0 \sqrt{\varepsilon_r \mu_r} )</td>
<td></td>
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</tbody>
</table>
Spinor representation of a field and construction of algorithm on basis MAS

\[ \Delta \times \vec{F} - k \vec{F} = 0 \]

Spinor basis

\[ \vec{r} = \begin{pmatrix} \vec{r}^r \\ \vec{r}^\ell \end{pmatrix} = \begin{pmatrix} \vec{r}^r + i \vec{r}^\ell \\ \vec{r}^r - i \vec{r}^\ell \end{pmatrix} \]

Spinor of electromagnetic field

\[ \vec{F} = \begin{pmatrix} \vec{F}^r \\ \vec{F}^\ell \end{pmatrix} = \begin{pmatrix} \vec{E} + i \eta \vec{H} \\ \vec{E} - i \eta \vec{H} \end{pmatrix} \]

Majorana-Dirac wave equation

Spinor representation of electromagnetic field

Fundamental Solution for biisotropic medium

\[ \vec{F}^{r,\ell}_n = \nabla \times \left( \hat{G}^n \cdot \vec{r}^n \right) \pm \frac{1}{k^{r,\ell}} \nabla \nabla \left( \hat{G}^n \cdot \vec{r}^n \right) \pm \hat{k} \cdot \left( \hat{G}^n \cdot \vec{r}^n \right) \]

Green function matrix

\[ \hat{G}^n = \begin{pmatrix} G^r_n & 0 \\ 0 & G^\ell_n \end{pmatrix} \]

Green function in free space

2D case

\[ G^{r,\ell}_n (\vec{r}, \vec{\rho}_n) = H^{(1)}_0 (k^{r,\ell} |\vec{r} - \vec{\rho}_n|) \]

3D case

\[ G^{r,\ell}_n (\vec{r}, \vec{r}_n) = \frac{1}{4\pi} \frac{e^{ik^{r,\ell} |\vec{r} - \vec{r}_n|}}{|\vec{r} - \vec{r}_n|} \]
The generalized Method of Auxiliary Sources (MAS)

Time dependence:

\[ e^{-i\omega t} \]

Wave equation:

\[ \nabla \times \bar{F} - k \bar{F} = 0 \]

Boundary condition:

\[ \hat{W} \bar{F}(\bar{r}) \bigg|_{\bar{r}=\bar{r}^s} = \bar{f}(\bar{r}^s), \quad M(\bar{r}^s) \in S \]

From the fundamental solutions of the Majorana-Dirac equations

\[ \Delta \times \bar{F}_n - k \bar{F}_n = \bar{r}_n \cdot \delta(\bar{r} - \bar{r}_n) \]

for the auxiliary points, we obtain a set of functions given by

\[ \{\bar{F}_n(\bar{r}, \bar{r}_n)\}_{n=1}^{\infty} \]

with radiation centers located at the auxiliary points \( \{\bar{r}_n\}_{n=1}^{\infty} \).

It has been proved that this set is complete and linearly independent in the function space \( \mathbf{L}^2 \). This allows us to obtain an approximate solution of the considered boundary problem from the superposition of \( N \) basis functions

\[ \bar{F}^{(N)}(\bar{r}) = \sum_{n=1}^{N} \hat{a}_n \bar{F}_n(\bar{r}, \bar{r}_n), \quad \bar{r} \in D, \quad \hat{a}_n = \begin{pmatrix} a_n^r & 0 \\ 0 & a_n^\ell \end{pmatrix} \]

where the expansion coefficients \( \{\hat{a}_n\}_{n=1}^{N} \) define the unknown amplitudes of the auxiliary spinor sources. Components of the scattered electromagnetic field are derived from spinor field using the simple relations

\[ \tilde{E}^{sc}(\bar{r}) = \tilde{E}_s^r + \tilde{E}_s^\ell = \frac{\eta^r}{\eta^r + \eta^\ell} \sum_{n=1}^{N} a_n^r \bar{F}_n^\ell(\bar{r}, \bar{r}_n) + \frac{\eta^\ell}{\eta^r + \eta^\ell} \sum_{n=1}^{N} a_n^\ell \bar{F}_n^r(\bar{r}, \bar{r}_n) \]

\[ \tilde{H}^{sc}(\bar{r}) = \tilde{H}_s^r + \tilde{H}_s^\ell = \frac{i}{\eta^r} \tilde{E}_s^r - \frac{i}{\eta^\ell} \tilde{E}_s^\ell \]

2D Periodic Green Functions

\[ \Pi(x, y) = \frac{1}{4i} \sum_{n=-\infty}^{\infty} \exp(i k n d \cos \theta) \cdot H_0^{(1)} \left( k \sqrt{(x - n d)^2 + y^2} \right) \]

\[ E_z = \sum_{n=-\infty}^{\infty} -\frac{kW_0}{4} \sqrt{\mu_0} \left[ \left( \frac{2\pi n}{d} \right)^2 - k^2 \right]^{-1/2} \cdot \exp \left[ -\left( x - x' \right)^2 \right]^{1/2} \left[ \left( \frac{2\pi n}{d} \right)^2 - k^2 \right]^{-1/2} \cdot \exp \left( \frac{i 2\pi ny}{d} \right) \]

\[ H_x = \sum_{n=-\infty}^{\infty} \frac{\pi n}{2kW_0 d} \left[ \left( \frac{2\pi n}{d} \right)^2 - k^2 \right] \cdot \exp \left[ -\left( x - x' \right)^2 \right]^{1/2} \left[ \left( \frac{2\pi n}{d} \right)^2 - k^2 \right]^{1/2} \cdot \exp \left( \frac{i 2\pi ny}{d} \right) \]

\[ H_y = \sum_{n=-\infty}^{\infty} -\frac{i}{4kW_0} \exp \left[ -\left( x - x' \right)^2 \right]^{1/2} \left[ \left( \frac{2\pi n}{d} \right)^2 - k^2 \right]^{1/2} \cdot \exp \left( \frac{i 2\pi ny}{d} \right) \]
3D Periodic Green Functions

\[ \Pi(x, y, z) = \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} \exp(iknd_x \cos \theta_x + ikmd_y \cos \theta_y) \frac{\exp \left( ik \sqrt{(x - nd_x)^2 + (y - nd_y)^2 + z^2} \right)}{ik \sqrt{(x - nd_x)^2 + (y - nd_y)^2 + z^2}} \]

Poisson Transformation

\[ \Pi(x, y, z) = -\frac{2\pi}{d_x d_y} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} \frac{1}{ik_p pq} \exp(ik_{xq} x + ik_{yp} y + ik_{zp} q) \exp \left( ik \sqrt{(x - nd_x)^2 + (y - nd_y)^2 + z^2} \right) \]

\[ k_{xq} = k \cos \theta_x + \frac{2\pi}{d_x} q, \quad k_{yp} = k \cos \theta_y + \frac{2\pi}{d_y} p, \quad h_p = \sqrt{k^2 - k_{yp}^2}, \quad p = 0, \pm 1, \pm 2, \ldots, q = 0, \pm 1, \pm 2, \ldots \]

\[ k_{zp} = \begin{cases} \sqrt{h_p^2 - k_{xq}^2}, & \text{if } h_p > k_{xq} \text{ and } k > k_{yp} \\ i \sqrt{k_{xq}^2 - h_p^2}, & \text{if } h_p < k_{xq} \text{ and } k > k_{yp} \end{cases} \]

\[ k_{zqp} = i \sqrt{h_p^2 + k_{xq}^2}, \quad \text{if } k < k_{yp} \]
MAS-MoM-Galerkin approach for general scattering problems

Triangulated surface of the scatterer

Triangulated auxiliary surface

MoM-like representation of current on the auxiliary surface

Current basis function and testing function

\[
\overline{J}(\vec{r}_s) \approx \sum_{n=1}^{N} I_n \overline{f}_n(\vec{r}_s), \quad \overline{f}_n(\vec{r}_s) = \begin{cases} 
\frac{l_n}{2A_n^+} \rho_n^+, & \text{if } \vec{r}_s \in T_n^+ \\
\frac{l_n}{2A_n^-} \rho_n^-, & \text{if } \vec{r}_s \in T_n^- \\
0, & \text{if } \vec{r}_s \notin T_n
\end{cases}
\]
Model-Based Parameter Estimation (MBPE)

In the frequency domain, the response of a system (for example refraction coefficient) may be optimally represented by a Cauchy’s method:

\[
F(s) = \frac{N(s)}{D(s)} + \text{Error}(s) = \sum_{i=0}^{n} N_i s^i + \text{Error}(s)
\]

\[
F(s) \sum_{i=0}^{d} D_i s^i - \sum_{i=0}^{n} N_i s^i = \text{Error}(s) \sum_{i=0}^{d} D_i s^i = E, \quad k = 1, \ldots, m
\]

where \(E\) is an unknown error vector. When \(F\) is known in \(m \geq n + d + 1\) points \(s_k D_d=1\)

\[
F(s) \sum_{i=0}^{d-1} D_i s^i - \sum_{i=0}^{n} N_i s^i = -F(s) s_d^d + E_k = R_k + E_k, \quad k = 1, \ldots, m
\]

\(E\) is zero when \(m = m_0 = n + d + 1\)

It is more reasonable to work with an overdetermined system of equations with \(m > m_0\).

For highly accurate MMP and MAS computations the overdetermination factor \(m/m_0=1.1\) is sufficient.

The adaptive MBPE procedure for filter analysis etc.

1. **Start**
2. Define *maximum order* 
   *Overdetermination factor* and *desired interval of changing parameter*
3. Construct data model; Solve system of linear equations for finding unknown coefficients $N_i$ and $D_i$; and estimate fitting error
4. **Fitting error** $< \varepsilon$ and $S \in [0, 1]$
   - **Yes**
   - **No**
5. Find frequency point for next calculation and carry out calculation for defined frequency point.
6. Increase order or divide domain into sub domains
7. **End**
MBPE procedure for fitting the filed response from dielectric cylinder

Procedure started from 5 uniformly distributed points and was finished after 16 iteration.
Field response of a dielectric cylinder

\[ \varepsilon = 10 \]
\[ r = 0.5m \]
2D metallic PhC slab modeled by MAS

The functions describing the fields of auxiliary sources should have the form:

\[ F_n \left( |\mathbf{r} - \mathbf{r}_n| \right) = \sum_{m=-\infty}^{+\infty} \alpha H_n^{(1)} \left( k \sqrt{(x-x_n-md)^2 + (y-y_n)^2} \right) \]

For the calculation of the reflected and transmitted fields for the 0 and \( p \)-th harmonic one has reflected \((y>y_n)\) and transmitted \((y<y_n)\) 0 and \( p \)-th harmonic:

\[ E_0 (x, y) = \sum_{n=1}^{N} a_n \exp \left( ik \cos \theta (x-x_n) \right) \exp \left( ik \left| \sin \theta \right| |y-y_n| \right) \]

\[ E_p (x, y) = \sum_{n=1}^{N} a_n \frac{\exp \left( i(k \cos \theta + g_p)(x-x_n) \right)}{h_p} \exp \left( ih_p |y-y_n| \right) \]

\[ g_p = \frac{2\pi}{d} p, \quad h_p = \frac{2\pi}{d} \sqrt{D^2 - (p + D \cos \theta)^2}, \quad D = \frac{d}{\lambda}, \quad (p = 0, \pm 1, \pm 2, \ldots) \]

Problem of coupled metallic nanoparticles

- Scattering Cross Section
- Silver Permittivity (Drude model)
- Frequency dependence of the permittivity of silver (Drude model).

The system contains two circular cylinders made of silver with a radius of 25nm and a surface-surface separation of 5nm. For the system response over the wavelength range 100nm to 350nm the adaptive MBPE algorithm requires only 63 frequency points for a maximum fitting error below 1%.

The Drude model was used for the frequency dependence of the permittivity of silver:

\[
e(\nu) = 1 + \frac{i\tau\omega_p^2}{2\pi\nu(1-i2\pi\nu)}
\]
2D metallic PhC slab modeled by MMP-MBPE, MAS-MBPE, and CST Microwave-Studio (FITD)

The PhC filter structure considered in the following consists of a 2D PhC with 5 layers of circular silver wires arranged on a square lattice. This structure extends to infinity in x direction and is finite in y direction. The wire radius is 73.3nm and lattice constant is 820nm. Ez polarization is considered.

The maximum difference between MMP and MAS is 0.02% and between MMP and FITD it is 0.1%. Only 20 points were computed by MMP and by MAS, the remaining points were interpolated by MBPE. The total computation time for these MBPE solutions was below 10 seconds on a PC.

MBPE for eigenvalue search

The lattice constant is $a$ and each primitive cell contains a circular metallic cylinder with radius $0.3a$. The background is vacuum and the relative permittivity of the cylinder is given by the Drude model of the metal.

The calculation started with 6 frequency points. Finally, only 25 frequency points were computed and the remaining points were interpolated by MBPE. The speed-up factor provided by the MBPE is more than 10.
Validation of the 2D and 3D Periodic Structure Algorithms

Validation 1. Half Space (comparison with Frenel formula)
Validation of the 2D and 3D Periodic Structure Algorithms

Validation 2. Dielectric Layer

![Diagram showing transmission and reflection of light through a dielectric layer]

- Incident light
- Reflected light
- Transmitted light
- Auxiliary sources
- Glass with refractive index $n=3.16$

Graph showing transmission as a function of thickness/wavelength:
- Analytical results
- Numerical results

Transmission values range from 0.55 to 1.00 with peaks at specific thickness/wavelength ratios.

Thiknes/wavelength: 0 to 2.5
Transmission: 0.55 to 1.00
Validation of the 2D and 3D Periodic Structure Algorithms

**Validation 3.** Comparison of 2D and 3D MAS approaches. Transmission coefficient per wavelength in units of period.
Double-periodic structure

![Graph showing transmission versus period/wavelength for a unit cell geometry with ε=10.](image)
Program package “FPC Simulator” has been developed to investigate and visualize wave propagation and scattering processes in finite photonic crystals of complex, composite materials. This package is a full analysis solution, providing a user with facilities for constructing the space lattice complicated configurations, specifying its material parameters, as well as calculating, post-processing and visualizing the desired characteristics of photonic crystals. Thus, the developed software ensures the best understanding of the undergoing processes in such devices.
The Geometry Edit dialog box
FDTD code for FPC modeling
FPC in 3D FDTD space

Lattice period $a=0.1\text{m}$

$\varepsilon=11.56$

Rode side=$0.36a$  Rode height=$24a$

$\lambda = 3a$

$R=0.37\%$
3D MAS code
Conclusion

- MAS-MoM extended for 3D periodic problems
- Periodic and double-periodic structures investigated
- MAS extended for 4-parametric dielectric (biisotropic) medium
- Adaptive MBPE algorithms added
- New FDTD code for FPC problems is under construction
Thank you for attention