



Research Networking Programmes

Short Visit Grant or Exchange Visit Grant

(please tick the relevant box)

Scientific Report

The scientific report (WORD or PDF file – maximum of eight A4 pages) should be submitted online within one month of the event. It will be published on the ESF website.

Proposal Title: Homogenized representation of metamaterials based on full-wave analysis for millimeter and submillimeter wave focusing system design

Application Reference N°: 4723

Scientific Report on the Research Activity within the framework of the ESF program entitled “New Frontiers in Millimetre/Sub-Millimetre Waves Integrated Dielectric Focusing Systems”

Author: Valentina Sozio

Scientific Advisors: Matteo Albani and Christophe Craeye

Date: November 2014

University of Siena
Department of Information
Engineering and Mathematics
Via Roma 56, 53100 Siena, Italy



Université catholique de Louvain
Information & Communication Technologies,
Electronics and Applied Mathematics Institute
Place du Levant 3, 1348 Louvain – La – Neuve, Belgium



1) Purpose of the visit

In recent years submillimeter wave focusing device design has benefited from new opportunities coming from the studies on metamaterials, artificial composite structures which exhibit novel properties not found in natural materials. The potential application of metamaterials in the imaging context was first suggested by Pendry with his idea of a “perfect lens” capable of focusing beyond the diffraction limit [1]. Subsequently, several groups have explored the possibility of subwavelength focusing using metamaterials.

The interaction of the electromagnetic radiation with metamaterials can be conveniently characterized using homogenization methods, which describe these structures as bulk homogeneous materials with certain effective parameters.

The applied electromagnetism group at the University of Siena has recently developed a method for the homogenization of reciprocal metamaterials [2]. So far, this approach has been applied in connection with the dual dipole approximation for the characterization of the embedded particles, i.e. microscopic electric and magnetic current distributions in the unit cell have been assumed to be described by a superposition of electric and magnetic dipole moments. The dual dipole approximation may provide satisfactory results, but it inherently introduces noncausal features into the electromagnetic interaction among the inclusions [3]. The proposed homogenization approach being general, more sophisticated methods, like integral-equation formulations, can be used for the description of the current distribution induced in the inclusions.

The research group at the Université catholique de Louvain has a long experience in full-wave analysis of periodic structures and in particular in the Method of Moment (MoM) technique for the simulation of structures made of complex elements, involving both metal and dielectric parts [4]. The purpose of the exchange visit was to use the full-wave analysis provided by MoM to characterize electromagnetic properties of 3D periodic arrays and exploit it within a homogenization method.

2) Description of the work carried out during the visit and main results obtained

In the following we show the idea that was developed to combine a Floquet based homogenization method and a full wave description of the induced currents in the inclusions via MoM.

Let us consider a 3D periodic array with one (or more) inclusion in the unit cell and let us assume the presence of an incident space harmonic electromagnetic field corresponding to the field radiated by impressed sources uniformly distributed all over the array with arbitrary space and time harmonic dependence. The microscopic field $\mathbf{E}(\mathbf{r})$, $\mathbf{H}(\mathbf{r})$ in the unit cell can be computed through MoM introducing equivalent electric and magnetic surface currents on the interfaces between the inclusion and the host medium. Moreover, by combining the Extinction and Love’s theorems (see Fig. 1), the microscopic field in the unit cell can be written as the sum of the field inside the inclusion and the field in the remaining volume of the cell. The use of the equivalence theorems allows one also to exploit the periodic Green’s function to compute the field inside the inclusions.

The homogenization method requires a spatial averaging of the microscopic fields as well as of the displacement vectors; as defined in [5], we take as averaged field \mathbf{E}_{av} , \mathbf{H}_{av} the zero-order

Floquet harmonic, and similar procedure leads to the averaged displacement vectors \mathbf{D}_{av} , \mathbf{B}_{av} such that it is possible to write the constitutive relations of the homogenized bianisotropic metamaterial as

$$\begin{aligned}\mathbf{D}_{av} &= \underline{\boldsymbol{\epsilon}}_{eff} \cdot \mathbf{E}_{av} + \underline{\boldsymbol{\zeta}}_{eff} \cdot \mathbf{H}_{av} \\ \mathbf{B}_{av} &= \underline{\boldsymbol{\mu}}_{eff} \cdot \mathbf{H}_{av} + \underline{\boldsymbol{\zeta}}_{eff} \cdot \mathbf{E}_{av}\end{aligned}\quad (2.1)$$

where $\underline{\boldsymbol{\epsilon}}_{eff}$, $\underline{\boldsymbol{\zeta}}_{eff}$, $\underline{\boldsymbol{\mu}}_{eff}$, $\underline{\boldsymbol{\zeta}}_{eff}$ are the effective constitutive parameters we are looking for.

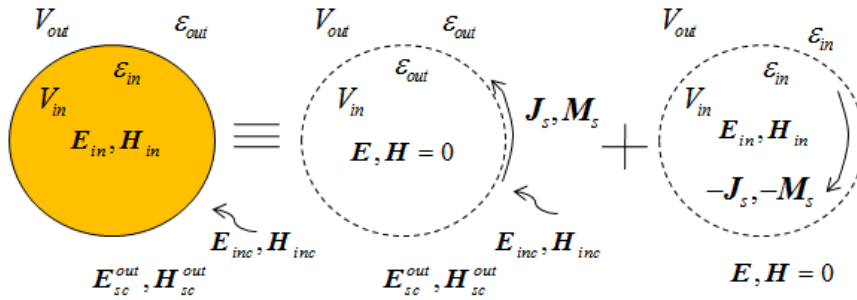


Fig. 1 Combination of the extinction and Love's theorem to define equivalent electric and magnetic currents at the surface of the object.

The method proposed would require the use of the 3D periodic Green's function in the MoM formulation to compute the equivalent electric and magnetic surface currents on the inclusions, but we tried to exploit another approach which is less cumbersome from a computational point of view and which has various advantages as explained later. The group of the Université catholique de Louvain has recently published an excellent work [6] in which an efficient surface integral equation method for the analysis of a finite stack of 2D periodic layers, containing any complex inclusion, is proposed. This approach is based on a double use of surface equivalence at inclusions level and at flat (possibly fictitious) interfaces between layers. The Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) formulation, which is based on the setting of the continuity of both the tangential electric and magnetic fields at the interface, is used to impose the boundary conditions. According to the method in [6], an equivalent electric and magnetic currents plane is inserted at every interface between layers. The equivalent currents on the planes sandwiching the layer isolate it from external sources, the unknowns related to the equivalent currents on the inclusions are eliminated from the final system of equations and the 2D periodic Green's function for an homogenous medium can be used.

Some further checks of the approach proposed in [6] for the structures under analysis were performed during the visit, by comparing the results provided by this method with those obtained with a commercial full-wave electromagnetic software. In particular, the distribution of the electric field on a x-y plane was compared.

Having as a final objective the development of the homogenization method, the preliminary idea was to extend this tool, available for a finite number of layers in one direction, to the analysis of a 3D infinitely periodic structure by imposing a further periodic boundary condition for the current densities on consecutive interfaces. By indicating with \mathbf{x}_i the vector of the equivalent electric and magnetic current densities on the i-th interface, we impose the quasi periodic condition between the current densities of two consecutive interfaces

$\mathbf{x}_{i+1} = \mathbf{x}_i e^{-j h \mathbf{k} \cdot \mathbf{z}}$, h being the thickness of the layer between the two interfaces. In this way, it is still possible to use the tool for a 2D periodic structure avoiding the calculation and/or tabulation of the 3D Green's function. In addition, the employment of equivalent currents at the interfaces between consecutive layers, preserves a limited number of MoM unknowns, associated with interfaces only. The use of the "interstitial" interface equivalent currents limits the study of the 3D infinite array to the analysis of two of its layers to determine the equivalent currents at the surface of the inclusions from which the microscopic and hence the averaged field and displacement vectors can be computed. The detailed formulas to arrive to (2.1) are omitted here for the sake of brevity.

The first necessary step was to check the validity of the extension of "interstitial" currents technique for the study of the 3D periodic metamaterial.

To do that we considered a quasi-periodic source distribution, i.e. a source distribution which is periodic according to a linear phase-shift $e^{-j h \mathbf{k} \cdot \mathbf{r}}$, exciting the 2D periodic structure with finite but large number of layers in the third dimension (here z). A simplified scheme of the structure is shown in Fig. 2. Note that the periodicity of the inclusions along x and y -direction is taken implicitly into account by using the 2D periodic Green's function when computing the MoM impedance matrices.

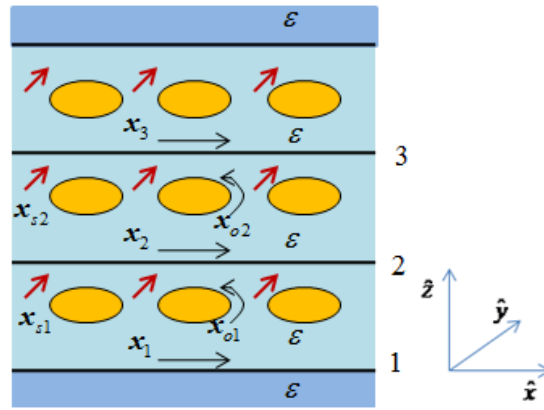


Fig. 2: Scheme of a finite stack of 2D-periodic layers of materials excited by a quasi-periodic source distribution

By applying the method developed in [6] to this problem, it is possible to find the interstitial currents on the interfaces of each layer in the finite stack. If the number of the layers is large enough the solution obtained for the currents in the finite stack case should converge to the solution in the case of a 3D infinite array. In the 3D periodic material the quasi-periodic source distribution can only excite Floquet modes with phase shifts between consecutive unit-cells identical to the phase shift of the excitation. Therefore the equivalent currents will have the same quasi-periodicity.

In the following we show the results related to a structure with 33 layers (34 interfaces) and one spherical dielectric inclusion in the unit cell. The comparison between the currents in the finite layered structure and the solution of the 3D infinite array has been performed in the

least square sense. In detail, we computed the following ratio $ratio_i = \frac{(\mathbf{x}_i)^{*T} \cdot \mathbf{x}_{inf}}{(\mathbf{x}_i)^{*T} \cdot \mathbf{x}_i}$ where \mathbf{x}_{inf} is

the solution in the infinite case and \mathbf{x}_i is the solution related to the i -th interface of the finite stack; then we reconstructed the currents densities in the 3D infinite structure case as

$\mathbf{x}_{\text{inf}}^{\text{rec}} = \text{ratio}_i \mathbf{x}_i$. In Fig. 3 we show the comparison of the solution in the infinite array case and the solution at interfacesn. 2, 5, 20, 25, 34 of the finite stack. As expected, we can observe that the currents in the finite structure case and the one of the infinite array case, are very close when we are far from the first and the last layers where the solution is affected by the truncation of the structure.

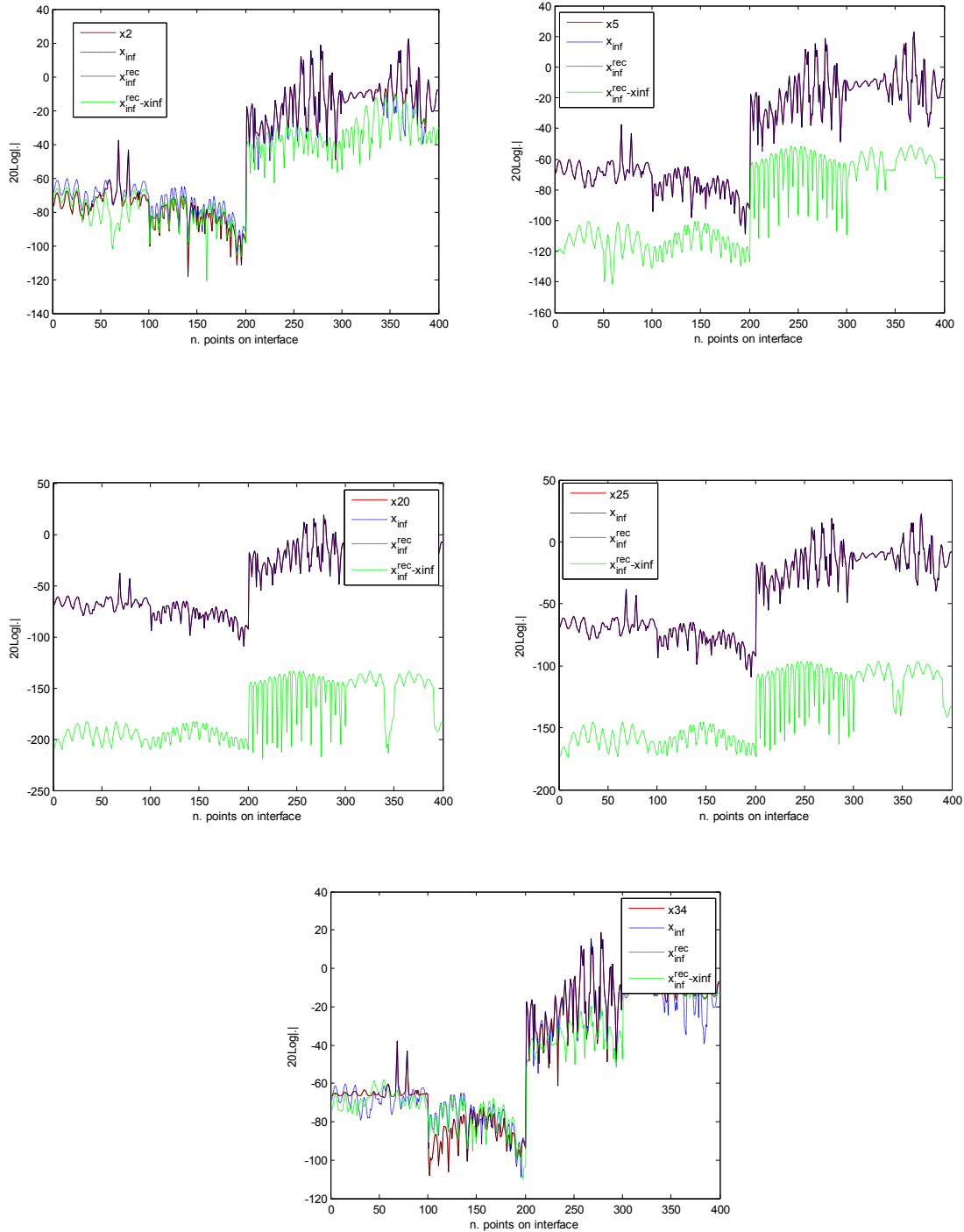


Fig. 3: Comparison between the solution for interstitial currents in the 3D periodic infinite structure and in the finite stack of the 2D periodic layers structure both excited by a quasi-periodic source distribution

These preliminary results have boosted the possibility to use the extended interstitial currents tool not only in the homogenization approach but also in the eigenmode analysis of the 3D infinite array. In fact to check the accuracy of an homogenization method, it is necessary to analyse the fundamental propagative modes of the material we want to homogenize. The study of the infinite structure can be limited to the analysis of two of its layers and the equation to be solved to find the eigenmodes of the composite material, obtained by imposing the continuity of tangential fields over an interface, is

$$-\left(\underline{\mathbf{Z}}_{pi,pi-1} - \underline{\mathbf{Z}}_{pi,o} \underline{\mathbf{Z}}_{o,o}^{-1} \underline{\mathbf{Z}}_{o,pi-1}\right) \mathbf{g}^{-1} \mathbf{x}_i + \left(\underline{\mathbf{Z}}_{pi,pi} - \underline{\mathbf{Z}}_{pi,o} \underline{\mathbf{Z}}_{o,o}^{-1} \underline{\mathbf{Z}}_{o,pi} - \underline{\mathbf{Z}}_{pi-1,o} \underline{\mathbf{Z}}_{o,o}^{-1} \underline{\mathbf{Z}}_{o,pi-1}\right) \mathbf{x}_i - \left(\underline{\mathbf{Z}}_{pi-1,pi} - \underline{\mathbf{Z}}_{pi-1,o} \underline{\mathbf{Z}}_{o,o}^{-1} \underline{\mathbf{Z}}_{o,pi}\right) \mathbf{g} \mathbf{x}_i = 0 \quad (2.2)$$

where $\underline{\mathbf{Z}}_{pi,pi}$ is the self-impedance MoM matrix of the i -th interface, $\underline{\mathbf{Z}}_{pi,pi-1}$, $\underline{\mathbf{Z}}_{pi-1,pi}$ the MoM impedance matrices describing the interaction between consecutive planes, $\underline{\mathbf{Z}}_{o,o}^{-1}$ the self-impedance matrix of the object, $\underline{\mathbf{Z}}_{pi,o}$, $\underline{\mathbf{Z}}_{pi-1,o}$, $\underline{\mathbf{Z}}_{o,pi-1}$, $\underline{\mathbf{Z}}_{o,pi}$, the impedance matrices related to the interaction between the plane above and below the object and the object itself, and $\mathbf{g} = e^{-j\mathbf{h}\mathbf{k}\cdot\hat{\mathbf{z}}}$.

From (2.2) a parabolic equation of the following form can be written

$$\underline{\mathbf{P}}(\mathbf{g}^2) \mathbf{x} = \mathbf{g} \mathbf{x} \quad (2.3)$$

Through (2.3) it is possible to find the eigenvalues \mathbf{g} , related to the wave vector \mathbf{k} describing the eigenmodes of the structure. Since the matrix $\underline{\mathbf{P}}(\mathbf{g})$ whose eigenvalues are computed depends on the result \mathbf{g} , solving the eigenvalues problem requires an iterative method and an exhaustive research on \mathbf{k} , and only one eigenvalue at a time can be found.

A sample example of the electric and magnetic eigen-currents of a 3D array structure with cylindrical inclusions analyzed with this method is shown in Fig. 4.

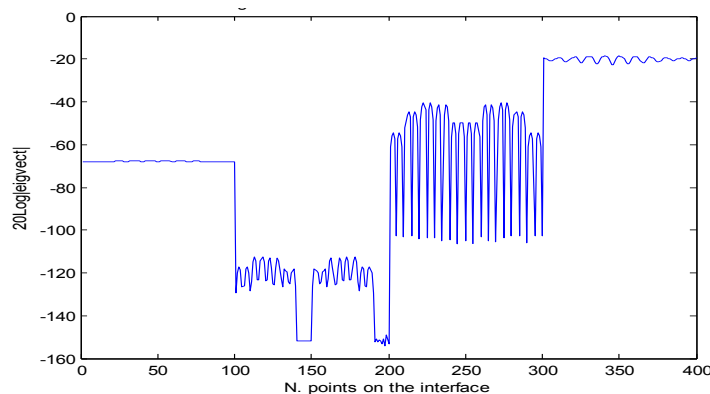


Fig. 4: Eigen-currents related to a 3D infinite array with one cylindrical inclusion in the unit-cell

A new technique has been then developed to linearize the eigenvalues problem and obtain an equation where the matrix, whose eigenvalues have to be found, is independent from them [7]. Moreover the big advantage of this novel technique is that the wave-vectors, corresponding to the found eigenvalues, can be computed in one operation. The technique consists of computing a modified self-impedance matrix for one interface which takes into account the

contribution of all the inclusions in the upper layers. The method is iterative and at each operation the number of upper layers included is doubled until reaching convergence. If the structure (host medium and/or inclusions) is lossy and the number of layers is large enough, this method allows one to write a linear eigen-equation. The scheme of the situation is illustrated in Fig. 5.

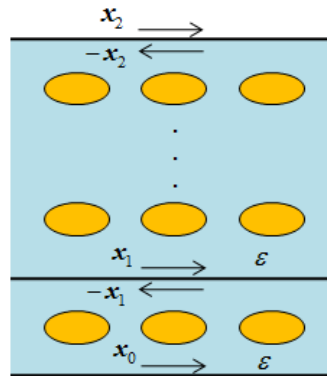


Fig. 5: Scheme simulated for the eigen-analysis of the 3D infinite array

For more details about the method formulation see [7].

The accuracy of the results obtained with this technique can be checked by comparing the eigenvector of the linearized formulation with the currents needed to ensure the continuity of the field at the interface (solution of the exact formulation given by (2.2)).

Some checks have been performed to verify that the continuity is ensured with excellent accuracy. Hence, the last two sources of errors in the result are related to the accuracy of the modified impedance matrix computation and to the MoM discretization of the problem.

3) Future collaboration with host institution

The study of the combination of the Floquet based homogenization method and the full wave description of the induced currents in the inclusions via MoM has reached a promising step. It needs however some further investigations which could certainly be the topic of future collaborations between the two involved research units.

4) Projected publications / articles resulting from the grant (ESF must be acknowledged in publications resulting from the grantee's work in relation with the grant)

Part of the activity carried out during the period of the exchange visit is resulted in an abstract which has been submitted to the 9th European Conference on Antennas and Propagation, titled "Efficient numerical analysis of 3D periodic metamaterials: multilayer approach and eigenmode analysis", with D. Tihon, V. Sozio, N.A. Ozdemir, M. Albani and C. Craeye as authors. Moreover the work realized during the exchange and its further developments may be presented during conferences in the next future and they may become the object of publications in international journals.

5) Other comments (if any) - Concluding Remarks

During the exchange visit a formulation and first studies for combining an homogenization method for 3D periodic metamaterials with a full wave description through MoM of the induced currents have been developed. An exact formulation for the analysis of the eigenmodes of the 3D infinite array, based on the PMCHWT formulation, has been elaborated and a new iterative technique to linearize the eigenvalues problem has been developed. Preliminary tests of the devised methods have given promising results.

6) References

- [1] J. B. Pendry, "Negative refraction makes a perfect lens," *Phys. Rev. Lett.*, vol 85, no.18, pp. 3966-3969, Oct. 2000.
- [2] A. Vallecchi, V. Sozio, M. Albani, and F. Capolino, "Generalized Lorentz-Lorenz method for the retrieval of plasmonic nanocluster metamaterial effective parameters," *Antennas and Propagation, 7th European Conference on*, Gothenburg, Sweden, pp.2994-2996, 8-12 April, 2013.
- [3] Alù, A. D. Yaghjian, R. A. Shore, and M. G. Silveirinha, "Causality relations in the homogenization of metamaterials," *Phys. Rev. B* 84, p. 054305, 2011.
- [4] N. Ozdemir, C. Craeye, K. Ehrhardt, A. Aradian, "Efficient integral equation approach for metamaterials made of core-shell nanoparticles at optical frequencies," *Proc. META2013 Conf.*, Dubai, March 18-22, 2013.
- [5] M. G. Silveirinha, "Metamaterial homogenization approach with application to the characterization of microstructured composites with negative parameters," *Phys. Rev. B*, vol. 75, p. 115104, 2007.
- [6] N.A. Ozdemir and C. Craeye, "An integral-equation method using interstitial currents devoted to the analysis of multilayered periodic structures with complex inclusions," submitted to *IEEE Transactions on Antennas and Propagation*, arXiv: 1408.3826v1, physics.optics, August 17, 2014.
- [7] D. Tihon, V. Sozio, N.A. Ozdemir, M. Albani and C. Craeye, "Efficient numerical analysis of 3D periodic metamaterials: multilayer approach and eigenmode analysis", *submitted to Antennas and Propagation, 9th European Conference*, 2015.