Homogenization process in nanotechnology and metamaterials

Homogenization is an important tool to solve complex problems composed of multiple elements with different properties. After homogenization of a system, a problem can be simplified to a single-element problem with a single effective value that takes into account the original heterogeneity of the problem. Such solution can be applied to many different physical and chemical problems.

One such example is the case of electromagnetism. From Maxwell equations, a single equation for Electric (E) and Magnetic (B) fields can be derived (Helmoltz equations) for the propagation of electromagnetic waves of frequency ω in vacuum, at a speed of *c*.

$$\left(\nabla^2 + \frac{\omega^2}{c^2}\right)E = 0 \quad ; \quad \left(\nabla^2 + \frac{\omega^2}{c^2}\right)B = 0$$

However, when waves propagate through a material, the electric and magnetic fields interact with its atoms. Typically, a cubic centimeter of any material contains around 10^{22} atoms inside, with their positive nuclei, and negative electrons. Solving the equation taking into account the interaction of such a high number of point charges is simply impossible, and thus a spatial and temporal homogenization is made to define effective macroscopic properties like dielectric constant (ε), magnetic permittivity (μ) and refraction index (n), as well as new variables like Displacement (D) and Magnetic Induction (H) fields which accounts for the interaction of the electromagnetic fields in the whole medium of propagation.

Nanotechnology has allowed us to artificially combine materials with these macroscopic properties. The propagation of waves through these new artificial mediums composed of different materials with different properties can also be simplified with a new homogenization process to yield new values for ε, μ and n, which in some cases can lead to exotic new phenomena like negative refraction or the apparition of bands where the propagation is not possible. Such is the case of metamaterials and photonic crystals.

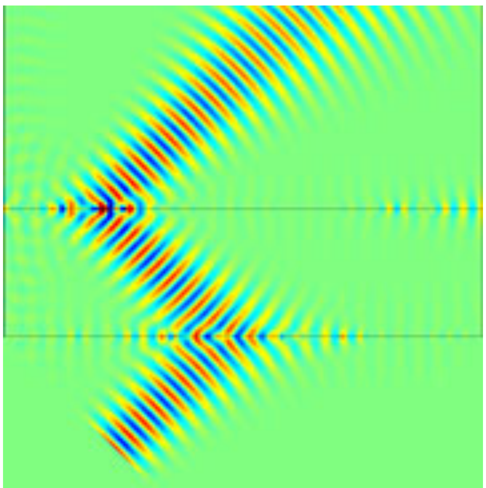


Figure 1. Example of negative refraction when light transmits through a metamaterial slab with a negative index of refraction

The possibility of design and fabrication of these new materials opens the path to the manipulation of light and its propagation that can be used in applications of security and defense.

Due to the different wavelengths that a single beam of light can transport, it becomes an important source of information of a scenario that can be exploited using sensors and detectors. Reconstruction of the spectrum of this light beam can for instance allow for the detection and identification of the presence of chemical warfare agents in the environment. For the separation of a light beam to obtain its spectrum, components that can filter and transmit extremely narrow bands are important, and can be achieved using photonic crystals.

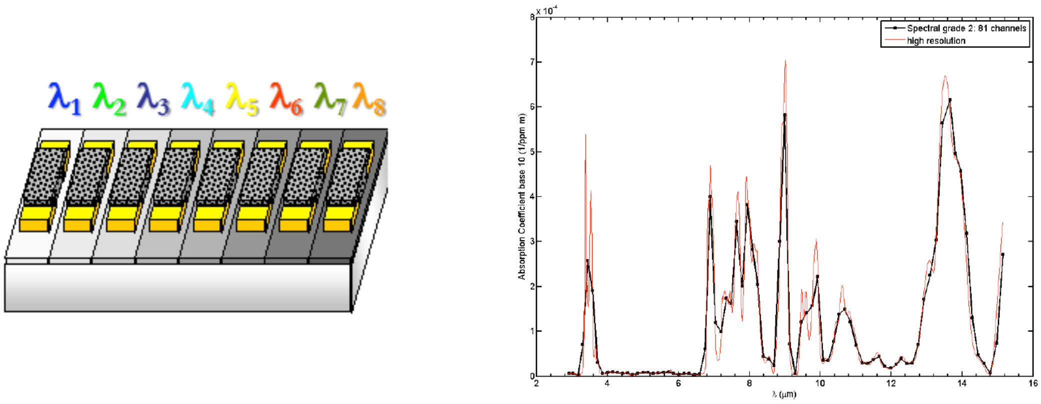


Figure 2. An array of sensors (left) combined with photonic crystals to produce a multispectral sensor allows the quick detection of the spectral signature of chemical warfare agents (right)

The opposite problem is avoiding the detection of a platform like an airplane, both in radar and infrared wavelengths. The use of metamaterials and transformation optics to design *'cloaking devices'*, becomes an important tool to help reducing the IR signature as well as the Radar Cross-Section.

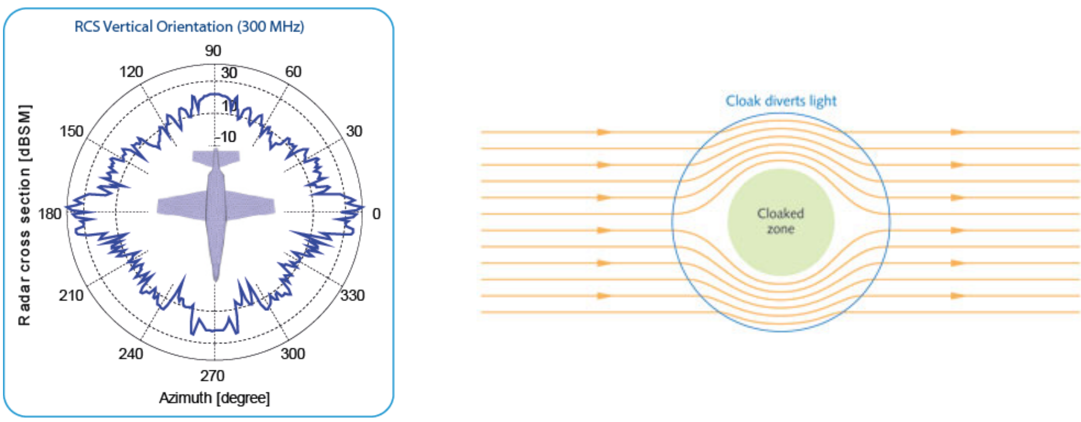


Figure 3. Left: Example of Radar Cross-Section measurement. Right: Schematic of a cloaking device that diverts light around an object.

Numerical experiments with COMSOL Multiphysics

Brief description of the study problem

The cloaking problem has given rise to a Hemholz equation after the homogenization of Maxwell's equations.

The importance of the homogenization is that it gives a tool to approximate our problem by one we can solve much more easily, and that gives us sufficient information. We pass to the limit in the way we don't study atoms individually, but rather the large structure properties.

There are a number of other contexts in which the homogenization of this type of equations appear. The following is a major example, which comes from Chemical Engineering. The advantage of this example is that it has been well studied from the theoretical point of view. The idea is to validate the homogenization as a tool, and show some of the computational advantages.

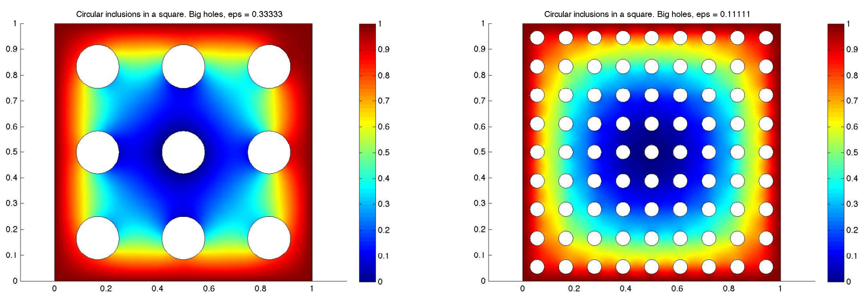
Consider particles of a catalyst material floating on a reactive solvent. The solvent diffuses in between the particles following a Laplace diffusion equation (known as Poisson's equation), a special case of Helmholz's equation (which is the one that actually appear on the metamaterial problem):

$$(-\Delta + k^2)u = f, \quad \Omega \tag{1}$$

in the case $k = 0$. On the boundary of the particles consider a nonlinear reaction

$$\frac{\partial u}{\partial n} + g(u) = 0 \tag{2}$$

The number of particles increases as the size of the generic particle decreases, and in the limit the system has become homogeneous. This process is called homogenization.



(a) Small number of particles

(b) Large number of particles

Figure 1: Example of how the number of particles grows

The solution of the above mention problems satisfies, after homogenization, a new equation, which is known as a semilinear elliptic equation

$$-\text{div}(A\nabla u) + \lambda g(u) = f, \quad \Omega \tag{3}$$

Objectives

- Numerical simulation of problems before and after homogenization with COMSOL Multiphysics (we will give an introductory course to COMSOL).
- Study of convergence of solutions to the solution of the homogenized problem.
- Comparison with the theoretical results (which we will be briefly presented by the organizer).
- Study the computation complexity of the problem as the number of particles involves increases, and compare computation times with the homogenized problem.