Internship proposition - Year 2018

Simulation of light absorption in nanostructured materials using a DGTD method formulated on non-conforming hybrid hexahedral/tetrahedral meshes

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Duration: 6 months

Monthly stipend: ≈ 500 €

Nanostructuring of materials has opened up a number of new possibilities for manipulating and enhancing light-matter interactions, thereby improving fundamental device properties. Low-dimensional semiconductors, like quantum dots, enable one to catch the electrons and control the electronic properties of a material, while photonic crystal structures allow to synthesize the electromagnetic properties. These technologies may, e.g., be employed to make smaller and better lasers, sources that generate only one photon at a time for applications in quantum information technology, or miniature sensors with high sensitivity. The incorporation of metallic structures into the medium add further possibilities for manipulating the propagation of electromagnetic waves. In particular, this allows subwavelength localisation of the electromagnetic field and, by subwavelength structuring of the material, novel effects like negative refraction, e.g. enabling super lenses, may be realized. Nanophotonics is the recently emerged, but already well defined field of science and technology, which aimes at establishing and using the peculiar properties of light and light-matter interaction in various nanostructures.

Numerical modeling of nanoscale light-matter interaction requires to solve the system of Maxwell equations possibly coupled to appropriate models of physical dispersion such as the Drude and Drude-Lorentz models. The Finite Difference Time-Domain (FDTD) method introduced by K.S. Yee in 1996 is a widely used approach for solving the resulting system of partial differential equations (PDEs). In this method, the whole computational domain is discretized using a structured (cartesian) grid. Due to the possible straightforward implementation of the algorithm and the availability of computational power, FDTD is often the method of choice for the simulation of time-domain nanoscale light-matter interaction problems. However, the space and time scales that characterize the underlying physical phenomena, in addition to the geometrical characteristics of the considered nanostructures, are particularly challenging for an accurate and efficient application of the FDTD method. During the last ten years, numerical methods formulated on unstructured meshes have drawn a lot of attention in computational electromagnetics with the aim of dealing with irregularly shaped structures and heterogeneous media. In particular, the discontinuous Galerkin time-domain (DGTD) method has progressively emerged as a viable alternative to the well established FDTD method.

NACHOS is a common project-team between Inria and the J.A. Dieudonné Mathematics Laboratory at University Nice Sophia Antipolis. The team gathers applied mathematicians and computational scientists who are collaboratively undertaking research activities aiming at the design, analysis, development and application of innovative numerical methods for systems of partial differential equations (PDEs) modeling nanoscale light-matter interaction problems. In this context, the team is developing the DIOGENeS software suite (https://diogenes.inria.fr/), which implements several Discontinuous Galerkin (DG) type methods tailored to the systems of PDEs modeling of time- and frequency-domain nanophotonics. In the time-domain case, the DGTD method is a discontinuous finite element type that relies on a high order interpolation of the electromagnetic field components within each cell of discretization mesh. This piecewise polynomial numerical approximation is allowed to be discontinuous from one mesh cell to another, and the consistency of the global approximation is obtained thanks to the definition of appropriate numerical traces for imposing the continuity of the tangential fields on faces shared by two neighboring cells. Time integration is achieved using an explicit scheme and, as a result of the discontinuity of the approximation, no global mass matrix inversion is required to advance the solution at each time step. Such a DGTD method, which is formulated on an unstructured tetrahedral mesh, has been designed in the context of the Ph.D thesis of Jonathan Viquerat for the simulation

of nanoscale light-matter interaction problems [Viq16]. This DGTD method has been recently refactored and implemented in the object-oriented framework of the DIOGENeS software suite.

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In this context, the objectives of this internship will be the following:

1. The preliminary implementation of the DGTD method capable of handling orthogonal hexahedral elements relies on Lagrange polynomial basis functions, as already done for tetrahedral elements in [Viq16]. The first objective will thus be to extend this implementation by considering an alternative basis expansion well suited for orthogonal hexahedral elements, leading to a diagonal or unitary local mass matrix. Preliminary validations will be performed by simulating a model electromagnetic wave propagation problem;
2. The second objective will be concerned with the ncessary algorithmic adaptations in order to obtained a DGTD method working on non-conforming hybrid hexahedral/tetrahedral meshes. This will include an auxiliary step aiming at the implementation of local refinement strategies of orthogonal hexahedral elements.
3. Finally, the third objective of this study will consist in the numerical validation and (accuracy and performance) evaluation of the developed DGTD method working on non-conforming hybrid hexahedral/tetrahedral meshes by considering test problems dealing with light absorption in nanostructured materials.

Required background:

- Master in applied mathematics or scientific computing;
- Knowledge of finite element type methods for solving PDE;
- Software development skills, preferably in Fortran 200x.

References

[FP13] C. Fisker and T.G. Pedersen. Opimization of imprintable nanostructured a-si solar cells: Fdtd study. *Opt. Expr.*, 21(S2):A208–A220, 2013. https://www.osapublishing.org/oe/fulltext.cfm?uri=oe-21-S2-A208&id=248432.

[LVD+14] R. Léger, J. Viquerat, C. Durochat, C. Scheid, and S. Lanteri. A parallel non-conforming multi-element DGTD method for the simulation of electromagnetic wave interaction with metallic nanoparticles. *J. Comp. Appl. Math.*, 270:330–342, 2014.

[Viq16] J. Viquerat. *Simulation of electromagnetic waves propagation in nano-optics with a high-order discontinuous Galerkin time-domain method*. PhD thesis, University Nice Sophia Antipolis, 2016. https://tel.archives-ouvertes.fr/tel-01272010.