In laser physics, gain or amplification is a process where the medium transfers part of its energy to an incident electromagnetic radiation, resulting in an increase in optical power. This is the basic principle of all lasers. Quantitatively, gain is a measure of the ability of a laser medium to increase optical power. Modeling optical gain requires to study the interaction of the atomic structure of the medium with the incident electromagnetic (EM) wave. Indeed, electrons and their interactions with electromagnetic fields are important in our understanding of chemistry and physics. In the classical view, the energy of an electron orbiting an atomic nucleus is larger for orbits further from the nucleus of an atom. However, quantum mechanical effects force electrons to take on discrete positions in orbitals. Thus, electrons are found in specific energy levels of an atom. In a semiclassical setting, such transitions between atomic energy levels are generally described by the so-called rate equations. These rate equations model the behavior of a gain material, and they need to be solved self-consistently with the system of Maxwell equations modeling EM wave (optical wave) propagation.

The interaction of EM wave radiation with a collection of atoms is characterized by two main features: (1) the effects of the medium on the field and (2) the change in the material parameters due to the incident field. When an EM wave propagates in a medium, the field induces a time varying dipole moment in the individual atoms that comprise the medium. The oscillating atoms lose energy through radiative and nonradiative mechanisms. The total field, which is the sum of the incident field and the fields radiated by the atoms, can thus be attenuated or amplified and phase-shifted by the medium. The effects of the medium on EM wave propagation can be modeled by suitably defining the polarization vector of the medium and solving the equation for the macroscopic polarization along with Maxwell’s equations. A classical example is given by the modeling of linear dispersive media for which one has to solve the system of time-domain Maxwell equations coupled to a set of linear ordinary differential equations (ODEs) (so-called, auxiliary differential equations - ADEs).

The ADE-based approach can also be adopted to model gain in lasers. The idea is to incorporates the atomic rate equations in the Maxwell-ADE framework. The rate equations describe the time evolution of the atomic energy level populations under the influence of applied signals. Since this model takes into account the effect of the propagating waves on the material parameters, it is capable of describing nonlinear gain and absorption effects and is valid over a large range of signal intensities. An ADE-FDTD method for solving this coupled model is proposed in [NY98]-[FKS10]. In the FDTD (Finite Difference Time-Domain) method [Yee66], 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 electromagnetic wave propagation problems. Besides, 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 accurately and efficiently with multiscale EM wave propagation problems. In particular, the discontinuous Galerkin time-domain (DGTD) method [HW02]-[FLLP05] has progressively emerged as a viable alternative to the well established FDTD method.

Our team at Inria 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 PDEs modeling nanoscale light-matter interaction problems. In this context, the team is developing the DIOGEneS software suite 1, 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 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

1https://diogenes.inria.fr/
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. An ADE-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 [Viq15]. This ADE-DGTD method has been studied theoretically in [LSV17]. It has
been implemented in the object-oriented framework of the DIOGENeS software suite, which is programmed
in Fortran 2008 and is adapted to high performance computing systems.

The general objective of the present internship is to design a DGTD method for solving the system of three-
dimensional time-domain Maxwell equations coupled to a four-level model of the optical gain similar to the one
studied in [FKS10]. As a first step, an ADE-DGTD method for this coupled system will be formulated as an
extension of the method introduced in [Viq15]. A stability study using an energy-based approach [LSV17] will
be conducted. Then, the proposed ADE-DGTD method will be implemented in the DIOGENeS framework,
and will be validated by considering test problems published in related works. This internship may be extended
as part of a PhD project depending on the availability of funds.

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Duration: 6 months
Monthly stipend: ≈ 600 €

Required background:
- Master in applied mathematics or scientific computing;
- Knowledge of finite element type methods for solving PDE;
- Knowledge of electromagnetics, Maxwell equations;
- Software development skills, preferably in Fortran 95/200x.

References


Galerkin time-domain method for the 3D heterogeneous Maxwell equations on unstructured meshes.


[LSV17] S. Lanteri, C. Scheid, and J. Viquerat. Analysis of a generalized dispersive model coupled to a


[Yee66] K.S. Yee. Numerical solution of initial boundary value problems involving Maxwell’s equations in