Second Workshop of the Math/Amsud Program

PHOTOM PHOTOvoltaic solar devices in Multiscale computational simulations

Inria Sophia Antipolis-Méditerranée, France

Kahn building, room K3

January 29 - February 1st, 2019

Abstract

This workshop is part of the collaborative Math/Amsud program and involves Brazilian, Chilean and French researchers in the field of applied mathematics, computational science and scientific computing. The general objective of the workshop is to kick off the Brazil-Chile-France PHOTOM project for taking full benefits of future developments, analysis, and high-performance implementations of innovative multiscale finite element methods for wave propagation models in grating media. This work is motivated by the use of multiscale numerical algorithms for the computational simulation of photovoltaic solar cells.

1 Summary of the Project

Solar energy is currently one of the main sources of clean energy and its importance has been growing up steadily in the last decades. Computational simulation of wave propagation in solar cells is crucial for the development of new photovoltaic devices. Modern solar cells embed complex multi-layer geometries that must be taken into account properly in numerical simulations. The new generation of parallel computers provides the necessary computational power to handle realistic three-dimensional wave propagation phenomena in complex multi-layer photovoltaic devices. Nevertheless, numerical methods must be revisited entirely to take full advantage of such new parallel facilities.

The PHOTOM project aims at devising, analysing and implementing innovative numerical algorithms, which are naturally prompt to be used in massively parallel computers, for the Helmholtz and the Maxwell equations. The physical coefficients contain highly heterogeneous and/or high contrast features in order to model wave propagation in grating media in view of the computational simulation of photovoltaic solar cells. The PHOTOM project corresponds to a two-year international collaboration between universities and research laboratories from Brazil, Chile and France. The researchers may be split in the following 3 fundamental themes (i) *Mathematical modelling of solar devices*; (ii) *Numerical schemes for PDE models*; (iii) *High-performance software systems*. coming from the LNCC - National Laboratory for Scientific Computing in Brazil, from Inria in France, and from PUCV - Pontifcia Universidad Catlica and UDEC - Universidad de Concepciòn in Chile.

2 Practical Informations

The Second PHOTOM meeting will take place at Inria Sophia Antipolis-Méditerranée, France [1].

3 Brazilian Participants

- Antonio Tadeu Gomes (LNCC)
- Weslley da Silva Pereira (LNCC)
- Frédéric Valentin (LNCC)

4 Chilean Participants

- Rodolfo Araya (UDEC)
- Diego Paredes (UDEC)
- Manuel Solano (UDEC)
- Patrick Vega (UDEC)

5 French Participants

- Théophile Chaumont-Frélet (Côte d'Azur University, Inria, CNRS, LJAD)
- Stéphane Descombes (Côte d'Azur University, Inria, CNRS, LJAD)
- Alexis Gobé (Côte d'Azur University, Inria, CNRS, LJAD)
- Mostafa Javadzadeh Moghtader (Côte d'Azur University, Inria, CNRS, LJAD)
- Zakari Kassali (Côte d'Azur University, Inria, CNRS, LJAD)
- Stéphane Lanteri (Côte d'Azur University, Inria, CNRS, LJAD)
- Georges Nehmetallah (Côte d'Azur University, Inria, CNRS, LJAD)
- Claire Scheid (Côte d'Azur University, CNRS, Inria, LJAD)

[1] https://www.inria.fr/en/centre/sophia

6 Program

- **January 29th**

9:00-9:30 Welcome coffee

9:30-10:00 Summary of Activities
Frédéric Valentin (LNCC) and Stéphane Lanteri (Inria)

10:00-10:40 New advances on MHM methods for Maxwell equations
Diego Paredes (UDEC)
The Multiscale Hybrid-Mixed method (or MHM for short), a finite element method, was presented in 2013 for solving the Laplace equation with a highly oscillatory permeability coefficient. This method appears as an attractive "divide-and-conquer" option to handle multiscale problems by naturally merging the effects of multiple scales to provide solutions with high-order precision on coarse meshes. Since our first work, this methodology was extended for several problems including Maxwell Equations, and new theoretical and computational features have been developed as a consequence. In this talk, we discuss some of these advances focusing on new discretization strategies its accuracy and computational performance.

10:40-11:00 Coffee Break

11:00-11:40 A posteriori error analysis of HDG methods
Patrick Vega (UDEC)
We introduce an analyze residual type a posteriori error estimators for a hybridizable discontinuous Galerkin (HDG) method applied to Stokes-type problems, establishing reliability and local efficiency of the estimators for the error in the natural norms, with constants written explicitly in terms of the physical parameters. We extend this to carrying out an a posteriori error analysis for HDG methods for equations arising from the simulation of photovoltaic solar cells, characterized by periodic diffraction gratings.

11:40-12:20 Multiscale Hybrid-Mixed method with local time-stepping strategy
Alexis Gobé (Inria)
The efficiency of explicit methods are always suffering when the considered geometries needs a high mesh refinement. One possibility is to use local time-stepping (LTS) methods in order to cluster our elements in different regions, each of them using its ideal time-step. The multiscale hybrid-mixed method (MHM) naturally handles this decomposition step. In this work, we investigate the possibility of having a local time stepping strategy for the MHM for Maxwell equations in heterogeneous media.

12:20-14:00 Lunch

14:00-16:00 Working session

16:00-16:30 End of 1st day

- **January 30th**

  9:30-10:00 Welcome coffee

  10:00-10:40 An HDG method for Maxwell's equations

  Manuel Solano (UDEC)

  The electromagnetic field in biperiodic diffraction grating structures can be calculated by solving Maxwell's equations with quasi-periodic boundary conditons on the vertical walls and radiation conditions above and below the structure. Towards the goal of analysing a hybridizable discontinuous Galerkin method for this problem, we begin with a simplified setting where perfect electric conductor boundary conditions are imposed on the whole boundary of the computational domain. We will present preliminary results and explain the main difficulties we are facing to achieve our goal.

  10:40-11:00 Coffee Break

  11:00-11:40 New results on the MHM method for wave propagation in complex media

  Weslley da Silva Pereira (LNCC)

  In this presentation, we will talk about new theoretical and numerical results regarding the MHM for elastic wave propagation problems. It covers the use of the MHM method on more general polytopal meshes, new theoretical results for wave propagation problems and numerical tests. We validate the MHM method by comparing it to the continuous Galerkin method in different scenarios and configurations. Notably, we use the highly heterogeneous media proposed in the HPC4e Test Suite [1] to show new results on both aligned and non-aligned meshes. We close the presentation discussing how the proposed technique extends to the time-dependent Maxwell equation on complex media.

  11:40-12:20 An explicit hybridizable discontinuous Galerkin method for the time-domain Maxwell equations

  Georges Nehmetallah (Inria)

  We present an explicit hybridizable discontinuous Galerkin (HDG) method for numerically solving the system of three-dimensional (3D) time-domain Maxwell equations. The method is fully explicit similarly to classical so-called DGTD (Dis continuous Galerkin Time-Domain) methods, is also high-order accurate in both space and time and can be seen as a generalization of the classical DGTD scheme based on upwind fluxes. We provide numerical results aiming at assessing its numerical convergence properties by considering a model problem. This method is a preliminary step for devising a hybrid explicit-implicit HDG method, so here we present a first strategy to construct such a method.

  12:20-14:00 Lunch

14:00-16:00 Working session

16:00-16:30 End of 2nd day

19h30 Dinner in Antibes

- **January 31st**

9:30-10:00 Welcome coffee

10:00-10:40 A general error analysis of the MHM method on non-conforming polyhedral meshes

Frédéric Valentin (LNCC)

This work revisits the general form of the Multiscale Hybrid-Mixed (MHM) method for the second-order Laplace equation under the perspective of non-convex non-conforming polyhedral meshes. In this context, we propose new stable multiscale finite elements such that they preserve the well-posedness, super-convergence and local conservation properties of the original MHM method under mild regularity conditions. Precisely, we show that piecewise polynomial of degree k-1 and k, where k is bigger or equal to 1, for the Lagrange multipliers along with continuous piecewise polynomial interpolations of degree k posed on second-level sub-meshes are stable if the latter is refined enough. Such one- and two-level discretization impact the error in a way that the discrete primal and dual variables achieve super-convergence in the natural norms under extra local regularity only. Numerical tests assess theoretical results.

10:40-11:00 Coffee Break

11:00-11:40 A Mutiscale Hybrid-Mixed method for the Helmholtz equation

Théophile Chaumont-Frélet (Inria)

11:40-12:00 Stability of Galerkin discretizations of Helmholtz problems with periodic boundary condition

Zakaria Kassali (Inria)

We present a novel multiscale finite element method for acoustic wave propagation in highly heterogeneous media which is accurate on coarse meshes. It originates from the primal hybridization of the Helmholtz equation at the continuous level, which relaxes the continuity of the unknown on the skeleton of a partition. As a result, face-based degrees of freedom drive the approximation on the faces, and independent local problems respond for the multiscale basis function computation. We propose a two-level version of the method when the basis functions are not promptly available, and we show how to recover other well-established numerical methods from it. A numerical analysis of the one-level MHM method establishes its well-posedness and prove the quasi-optimality for the numerical solution. Also, we demonstrate that the MHM method is super convergent in the natural norms. We assess theoretical results, as well as the performance of the method on heterogeneous domains, through a sequence of numerical tests.

12:20-14:00 Lunch

14:00-16:00 Working session

16:00-16:30 End of 3rd day

- **February 1st**

9:30-10:00 Welcome coffee

10:00-10:40 Using DSL concepts and C++11 language to develop flexible, high-performance FEM solvers based on the family of MHM methodsTitle
Antonio Tadeu Gome (LNCC)
In this talk, we discuss about the use of domain-specific language (DSL) concepts for the development of high-performance FEM solvers. Such an approach has already been used elsewhere: FreeFEM++, FEniCS and Firedrake are well-known examples. Theses approaches, however, either depend on the availability of specific-purpose runtime engines to support the DSL execution (e.g. FreeFEM++), or use glue language engines to express the DSL constructs (e.g. FEniCS and Firedrake, both of which use Python as the glue language). We argue that these approaches impose unnecessary burden on their users, in particular in HPC environments, because these users need to deploy additional software packages that may complicate maintenance and evolution of their products, and also need to learn new language constructs that may increase the time-to-market of their products. We propose an approach fully-based on C++11 to develop high-performance FEM solvers. Our approach is based on the exploration of general design patterns such as the Visitor Pattern, as well as C++-specific design patterns such as the Expression Template Pattern and the Curiously-Recurring Template Pattern seasoned with new C++11 constructs such as perfect forwarding. The objective is to express variational formulations that can be symbolically evaluated at compile-time and numerically evaluated at runtime, thus rendering both efficient and expressive FEM codes. Our approach is inspired by C++ libraries acting at the linear algebra level, such as Boost uBlas and Eigen. Our approach has been used for implementing a software library that supports the family of Multiscale Hybrid-Mixed (MHM) methods. In this talk we present the details about our approach as well as some numerical experiments that evaluate its performance.

10:40-11:00 Coffee Break

11:00-11:40 HDG method for the 3d frequency-domain Maxwell's equations with application to nanophotonics

Mostafa Javadzadeh Moghtader (Inria)

HDG method is a new class of DG family with significantly less globally coupled unknowns, and can leverage a post-processing step to gain super-convergence. Its features make HDG a possible candidate for computational electromagnetics applications, especially in the frequency- domain. The HDG method introduces an hybrid variable, which represents an additional unknown on each face of the mesh, and leads to a sparse linear system in terms of the degrees of freedom of the hybrid variable only. Our HDG method had been first introduced for the system of 3d time-harmonic Maxwells, combined to an iterative Schwarz domain decom- position (DD) algorithm to allow for an efficient parallel hybrid iterative-direct solver. The resulting DD-HDG solver has been applied to classical applications of electromagnetics in the microwave regime. In the present contribution, we further focus on this particular physical context and propose a arbitrary high order HDG method for solving the system of 3d frequency-domain Maxwell equations coupled to a generalized model of physical dispersion in metallic nanostructures at optical frequencies. Such a generalized dispersion model unifies most common dispersion models, like Drude and Drude-Lorentz models, and it permits to fit large range of experimental data. The resulting DD-HDG solver is capable of using different element types and orders of approximation, hence enabling the possibilities of p-adaptivity and non-conforming meshing, and proves to have interesting potentials for modeling of complex nanophotonic and nanoplasmonic problems.

11:40-12:20 Future perspectives and summary of the workshop

12:20-14:00 Lunch

14:00-14:30 End of workshop

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