2019-02128 - Post-Doctoral Research Visit F/M
Computation of electromagnetic quasi-normal modes in nanostructures using contour integration techniques

**Contract type:** Fixed-term contract  
**Level of qualifications required:** PhD or equivalent  
**Function:** Post-Doctoral Research Visit  
**Level of experience:** From 3 to 5 years

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**About the research centre or Inria department**

The Inria Sophia Antipolis - Méditerranée center counts 34 research teams as well as 8 support departments. The center's staff (about 500 people including 300 Inria employees) is made up of scientists of different nationalities (250 foreigners of 50 nationalities), engineers, technicians and administrative staff. 1/3 of the staff are civil servants, the others are contractual agents. The majority of the center's research teams are located in Sophia Antipolis and Nice in the Alpes-Maritimes. Four teams are based in Montpellier and two teams are hosted in Bologna in Italy and Athens. The Center is a founding member of Université Côte d'Azur and partner of the I-site MUSE supported by the University of Montpellier.

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**Context**

This postdoctoral project will be conducted in the Nachos project-team at the Inria Sophia Antipolis-Méditerranée research center, in close collaboration with researchers from the HiPacs project-team at the Inria Bordeaux - Sud-Ouest research center.

**Nachos** is a joint project-team between Inria and the Jean-Alexandre 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 time- and frequency-domain Maxwell equations possibly coupled to differential equations modeling the behaviour of propagation media at optical frequencies. DIOGENes is a unique numerical framework leveraging the capabilities of DG techniques for the simulation of multiscale problems relevant to nanophotonics and nanoplasmonics.

**HiPacs** is a joint project-team with Bordeaux INP, Bordeaux University and CNRS (LaBRI UMR 5800). The overarching objective of the activities of the team is to perform efficiently front-end simulations arising from challenging research and industrial multiscale applications. The solution of these challenging problems require a multidisciplinary approach involving applied mathematics, computational and computer sciences. In applied mathematics, it essentially involves advanced numerical schemes. In computational science, it involves massively parallel computing and the design of highly scalable algorithms and codes to be executed on emerging extreme scale platforms. Through this approach, HiPacs intends to contribute to all steps that go from the design of new high-performance more scalable, robust and more accurate numerical schemes to the optimized implementations of the associated algorithms and codes on very high performance supercomputers. A central topic of the team is high performance solvers for linear algebra problems including sparse direct solver for heterogeneous platforms, hybrid direct/iterative solvers based on algebraic domain decomposition, linear Krylov solvers and eigensolvers.

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**Assignment**

The recent advances of nanoscale fabrication techniques have enabled the design and manufacture of deep subwavelength structures that interact with light in exceptional ways. Such nanostructures are used as building blocks of a new generation of nanophotonic devices, such as, for instance, photovoltaic cells for solar energy harvesting or microLEDs for efficient light extraction. Numerical simulations are very helpful to better understand the properties of these nanostructures, and improve their efficiency. In
practice, nanoscale light-matter interactions can be studied by considering the system of Maxwell equations with suitable models of physical dispersion in materials (e.g., metals and semiconductors). The design of accurate and efficient numerical methods and the development of scalable solvers for these PDE models, which are capable of dealing with large-scale three-dimensional nanophotonic devices, is of paramount importance.

In this context, the development of modal-type solvers based on so-called Quasi-Normal Modes (QNMs) for the study of resonant features of nanophotonic and plasmonic devices is receiving an increasing interest [1]. Indeed, once computed, QNMs can be combined to recover a nanostucture response in a large frequency range. However, computing QNMs is a computationally expensive task, which amounts to solving a (sometimes non-linear) generalized eigenvalue problem for the underlying PDE model. Promising approaches to solve this problem, which we will consider in this postdoctoral project, are based on Contour Integration (CI) techniques [2]-[3]. Contrary to traditional approaches that rely on well-established numerical linear algebra techniques for the computation of eigenvalues and eigenvectors of the matrix operator resulting from a mesh-based discretization of the underlying PDE model, in the CI formalism, one uses complex contour integration to calculate the eigenvectors associated with eigenvalues that are located inside some user-defined region in the complex plane. One attractive feature of this approach is that it naturally induces a parallel process by dividing the complex plane into a collection of disjoint regions where eigenpairs can be computed concurrently.

Main activities

In this postdoctoral project we will combine the expertise and knowhow of two Inria project-teams. The Nachos project-team of the Inria Sophia Antipolis-Méditerranée research center designs and develops fullwave solvers for nanoscale light-matter interactions, which are based on high order discontinuous Galerkin methods. The methodological contributions of the team are materialized in the DIOGENes [https://diogenes.inria.fr] software suite, which is dedicated to computational nanophotonics. Several high order discontinuous Galerkin methods are implemented in this software suite for solving the PDE models in time-domain [4] and frequency-domain [5] settings. The Hiepac project-team of Inria Bordeaux - Sud-Ouest designs and develops scalable numerical linear algebra solvers for general large sparse linear matrix systems. The methodological contributions of the team are materialized in the MaPhyS [https://gitlab.inria.fr/solverstack/maphys] algebraic domain decomposition solver and in the Fabulous [https://gitlab.inria.fr/solverstack/fabulous] versatile and flexible library that implements block Krylov iterative methods for the solution of linear systems of equations with multiple right-hand sides.

The postdoctoral fellow will be in charge of investigating, implementing and assessing different techniques to compute QNMs of three-dimensional nanostructures. He will in particular study the FEAST algorithm [3] and Beyn’s approach [2]. He will rely on the frequency-domain DG solver [5], the MaPhyS algebraic domain decomposition solver and numerical linear algebra methods from the Fabulous library for the design of high performance tools for the computation of QNMs. After validating his initial implementations of these tools on synthetic examples, he will develop a new component of the DIOGENes software suite, which will be dedicated to the computation and exploitation of QNMs for the analysis of large-scale nanophotonic devices.


Skills

Candidates must hold a PhD degree in applied mathematics or scientific computing.

Required knowledge and skills are: a sound knowledge of numerical analysis and development of finite element type methods for solving PDEs and numerical linear algebra techniques; a concrete experience in numerical modeling for computational electromagnetics; strong software development
skills, preferably in Fortran 95/2008; a first experience with programming models for high performance computing systems.

A previous research experience in computational nanophotonics will clearly be an asset for this position.

Benefits package
- Subsidized meals
- Partial reimbursement of public transport costs
- Leave: 7 weeks of annual leave + 10 extra days off due to RTT (statutory reduction in working hours) + possibility of exceptional leave (illness, moving home, etc.)
- Possibility of teleworking (after 6 months of employment) and flexible organization of working hours
- Professional equipment available (videoconferencing, loan of computer equipment, etc.)
- Social, cultural and sports events and activities
- Access to vocational training
- Social security coverage

Remuneration
Gross Salary: 2653 € per month