

Offer #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

Fonction: Post-Doctoral Research Visit Level of experience: From 3 to 5 years

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 320 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.

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 Hiepacs 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.

Hiepacs is a joint project-team with Bordeaux INP, Bordeaux University and CNRS (LaBRI UMR 5800). The overarching objectiveof the activities of the team is to perform efficiently frontier 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, Hiepacs 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 veryhigh 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 eignesolvers.

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 nanostructure 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 [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 PDE models in time-domain [4] and frequency-domain [5] solving the settings. The Hiepacs 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 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 forthe 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.

- [1] P. Lalanne, W. Yan, K. Vynck, C. Sauvan, and J.P. Hugonin, Light interaction with photonic and plasmonic resonances, Las. Phot. Rev. 12 (2018), 1700113.
- [2] W.J. Beyn, An integral method for solving nonlinear eigenvalue problems, Lin. Alg. Appl. 236 (2012), 3839–3863.
- [3] B. Gavin, A. Miedlar, and E. Polizzi, FEAST eigensolver for nonlinear eigenvalue problems, J. Comput. Sci. 27 (2018), 107–117.
- [4] S. Lanteri, C. Scheid, and J. Viquerat, Analysis of a generalized dispersive model coupled to a DGTD method with application to nanophotonics, SIAM J. Sci. Comp. 39 (2017), no. 3, 831–859.
- [5] L. Li, S. Lanteri, and R. Perrussel, A hybridizable discontinuous Galerkin method com- bined to a Schwarz algorithm for the solution of 3d time-harmonic Maxwell's equations, J. Comput. Phys. 256 (2014), 563–581.

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 exprience 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 (sick children, 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

General Information

 Theme/Domain: Numerical schemes and simulations Scientific computing (BAP E)

• Town/city: Sophia Antipolis

• Inria Center : Centre Inria d'Université Côte d'Azur

Starting date: 2020-04-01
Duration of contract: 12 months
Deadline to apply: 2020-12-31

Contacts

• Inria Team: NACHOS

• Recruiter:

Lanteri Stéphane / Stephane.Lanteri@inria.fr

About Inria

Inria is the French national research institute dedicated to digital science and technology. It employs 2,600 people. Its 200 agile project teams, generally run jointly with academic partners, include more than 3,500 scientists and engineers working to meet the challenges of digital technology, often at the interface with other disciplines. The Institute also employs numerous talents in over forty different professions. 900 research support staff contribute to the preparation and development of scientific and entrepreneurial projects that have a worldwide impact.

Warning: you must enter your e-mail address in order to save your application to Inria. Applications must be submitted online on the Inria website. Processing of applications sent from other channels is not guaranteed.

Instruction to apply

Defence Security:

This position is likely to be situated in a restricted area (ZRR), as defined in Decree No. 2011-1425 relating to the protection of national scientific and technical potential (PPST). Authorisation to enter an area is granted by the director of the unit, following a favourable Ministerial decision, as defined in the decree of 3 July 2012 relating to the PPST. An unfavourable Ministerial decision in respect of a position situated in a ZRR would result in the cancellation of the appointment.

Recruitment Policy:

As part of its diversity policy, all Inria positions are accessible to people with disabilities.