Inria

Offer #2024-07083

PhD Position F/M Deep Neural Network-assisted computational design of highly efficient ultrafast dynamical metasurfaces

Contract type : Fixed-term contract

Level of qualifications required : Graduate degree or equivalent

Other valued qualifications : Master or engineering degree in numerical mathematics or scientific computing

Fonction : PhD Position

Level of experience : Recently graduated

About the research centre or Inria department

The Inria centre at Université Côte d'Azur includes 37 research teams and 8 support services. The centre's staff (about 500 people) is made up of scientists of different nationalities, engineers, technicians and administrative staff. The teams are mainly located on the university campuses of Sophia Antipolis and Nice as well as Montpellier, in close collaboration with research and higher education laboratories and establishments (Université Côte d'Azur, CNRS, INRAE, INSERM ...), but also with the regiona economic players.

With a presence in the fields of computational neuroscience and biology, data science and modeling, software engineering and certification, as well as collaborative robotics, the Inria Centre at Université Côte d'Azur is a major player in terms of scientific excellence through its results and collaborations at both European and international levels.

Context

The present doctoral project is part of a collaborative project between the Atlantis project-team from the Inria Research Center at Université Côte d'Azur and the CNRS-CRHEA laboratory in Sophia Antipolis, France.

Atlantis is a joint project-team between Inria and the Jean-Alexandre Dieudonné Mathematics Laboratory at Université Côte d'Azur. 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) modelling nanoscale light-matter interaction problems. In this context, the team is developing the DIOGENeS [https://diogenes.inria.fr/] software suite, 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.

The Research Center for Heteroepitaxy and its Applications (CRHEA) is a CNRS research laboratory. The laboratory is structured around the growth of materials by epitaxy, which is at the heart of its activities. These materials are grouped today around the theme of high bandgap semiconductors: gallium nitrides (GaN, InN, AlN and alloys), zinc oxide (ZnO) and silicon carbide (SiC). Graphene, a zero bandgap material, epitaxially grown on SiC, completes this list. Different growth methods are used to synthesize these materials: molecular beam epitaxy (under ultrahigh vacuum) and various vapor phase epitaxies. Structural, optical and electrical analysis activities have been organized around this expertise in epitaxy. The regional technology platform (CRHEATEC) makes it possible to manufacture devices. In terms of applications, the laboratory covers both the field of electronics (High Electron Mobility Transistors, Schottky diodes, tunnel diodes, spintronics, etc.) and that of optoelectronics (light-emitting diodes, lasers, detectors, materials for nonlinear optics, microcavity structures for optical sources, etc.). The laboratory has also embarked on the "nano" path, including both fundamental aspects (nanoscience) and more applied aspects (nanotechnology for electronics or optics).

Assignment

Metasurfaces are engineered materials that can precisely control the behavior of electromagnetic waves by using subwavelength-sized elements called meta-atoms. These meta-atoms can be designed to exhibit specific electromagnetic responses, which allows metasurfaces to manipulate the properties of light waves in a highly controlled manner. Metasurfaces can be divided into two main categories: passive and active. Passive metasurfaces have a fixed response to incident electromagnetic waves, meaning that their functionality is set during fabrication and their geometrical parameters are tuned to achieve the desired response. Active metasurfaces, on the other hand, can actively change their response in real-time by incorporating active materials such as phase change materials, liquid crystals, or materials with electro-optical response. This allows for dynamic manipulation of light waves upon the application of external stimuli, achieved by spatially modulating the permittivity of the nano-resonators. However, designing efficient active metasurfaces is challenging because the refractive index modulation response is often not sufficient to achieve the necessary conditions for wavefront control, especially for materials with ultrafast response. This usually requires a deep understanding of the topological resonance behavior and careful numerical modeling to achieve full phase modulation with high amplitude response in a single unit-cell configuration.

The main goal of this PhD project is to use numerical methods to optimize the design of active nanostructures in order to achieve the highest possible phase modulation and amplitude response. The optimization process will focus on adjusting the dimensions and shapes of meta-atoms and will take into account the characteristics of the active materials used. For passive metasurfaces, different resonators with different shapes are used to achieve the desired phase profile, but in an active system, all resonators in a microcell will have the same shape but will be modulated differently by applying different voltages [MELS23]. As a result, a more advanced computational design methodolgy is needed to account for the effects of near-field coupling and fabrication errors.

For passive metasurfaces, we have developed a numerical methodology that has previously been used successfully for desiging metadeflectors and metalenses [MELS19, MELS21]. This method consists of two components: a global optimization method based on statistical learning for the outer loop, and a fullwave solver for the inner loop to accurately evaluate a given design. The outer loop, which is driven by the Efficient Global Optimization (EGO) method, explores the predefined design space in an efficient manner to minimize the number of calls to the fullwave solver. The inner loop relies on the Discontinuous Galerkin Time-Domain (DGTD) method, which combines high order discontinuous finite elements for space discretization with an explicit time-stepping method for time integration of the 3D time-domain Maxwell equations. The DGTD method [Viq15] is accurate, efficient and easy to implement. Although it is a powerful and flexible inverse design approach, tackling the modeling challenges of actives metasurfaces requires to address carefully the computatoinal efficiency issues.

Beside the above-mentioned high-fidelity DGTD electromagnetic solver, we are also actively studying reduced-order modeling (ROM) strategies in the context of time-domain electromagnetics by studying the applicability of the proper orthogonal decomposition (POD) method. In this ROM approach, a reduced subspace with a significantly smaller dimension is constructed by a set of POD basis vectors extracted offline from snapshots that are extracted from simulations with a high order DGTD solver. In particular, a non-intrusive POD-based ROM has been developed for the solution of parameterized time-domain electromagnetic scattering problems where considered parameters are the electric permittivity and the temporal variable [LHLL21]. Although this non-intrusive POD-based ROM method introduced in provides encouraging results, it is not as efficient and robust as one would expect and it does not allow to account for a parametrized geometry. In particular, the hyperbolic nature of the underlying PDE system, i.e., the system of time-domain Maxwell equations, is known to represent a challenging issue for linear reduction methods such as POD. In practice, a large number of modes is required therefore hampering the obtention of an efficient ROM strategy. One possible path to address this problem which is currently investigated by several groups worldwide relies on nonlinear reduction techniques that leverage Artificial Neural Networks (ANNs) [PMH23]-[FM22]-[DH23]. The main objective of the present PhD project will be to investigate and develop such an ANN-assisted ROM strategy for the particular modeling context of active metasurfaces. This will require extending the approach previously proposed in [LHLL21] by addressing (1) the specificities of electrically-driven active metasurfaces and (2) the efficient integration of the developed ANN-based ROM strategy in an inverse design workflow similar to the ones described in [MELS19, MELS21].

[MELS19] M. Elsawy, S. Lanteri, R. Duvigneau, G. Brière, M.S. Mohamed and P. Genevet, *Global optimization of metasurface designs using statistical learning methods*, Scientific Reports, Vol. 9, No. 17918, (2019)

[MELS21] M. Elsawy, A. Gourdin, M. Binois, R. Duvigneau, D. Felbacq, S. Khadir, P. Genevet an S. Lanteri, *Multiobjective statistical learning optimization of RGB metalens*, ACS Photonics, Vol. 8, No. 8, pp. 2498–2508 (2021)

[MELS22] M. Elsawy, M. Binois, R. Duvigneau, S. Lanteri, and P. Genevet, *Optimization of metasurfaces under geometrical uncertainty using statistical learning*, Optics Express, Vol. 29, No. 19, pp. 29887–29898 (2021)

[MELS23] M. Elsawy, C. Kyrou, E. Mikheeva, R. Colom, J-Y Duboz, K. Zangeneh Kamali, D. Neshev, S. Lanteri and P. Genevet, *Universal active metasurfaces for ultimate wavefront molding by manipulating the reflection singularities,* Laser & Photonics Reviews, Vol. 17, No. 7, Art. No. 2200880 (2023)

[LHLL21] K. Li, T.-Z. Huang, L. Li and S. Lanteri, *Non-intrusive reduced-order modeling of parameterized electromagnetic scattering problems using cubic spline interpolation,* Journal of Scientific Computing, Vol. 87, No. 52 (2021)

[PMH23] F. Pichi, B. Moya and J.S. Hesthaven. A graph convolutional autoencoder approach to model order reduction for parametrized PDEs. arXiv:2305:08573v1 (2023)

[FM22] S. Frescal and A. Manzoni. *POD-DL-ROM: enhancing deep learning-based reduced order models for nonlinear parametrized PDEs by proper orthogonal decomposition.* Computer Methods in Applied Mechanics and Engineering, Vol. 388, pp. 114181 (2022)

[DH23] J. Duan and J.S. Hesthaven. *Non-intrusive data-driven reduced-order modeling for time-dependent parametrized problems.* Journal of Computational Physics, Vol. 497, pp. 112621 (2023)

[Viq15] J. Viquerat, *Simulation of electromagnetic waves propagation in nano-optics with a high-order discontinuous Galerkin time-domain method,* Ph.D. thesis, University of Nice-Sophia Antipolis (2015)

Main activities

- Bibliography study on existing ANN-based ROM methods
- Formulation of an ANN-based ROM method for time-domain nanophotonics in the context of electrically-driven active metasurfaces
- Development (in Fortran 2003 and Python) of the method for 3d problems
- Detailed assessment of the novel ANN-based ROM method by considering model problems
- Formulattion and development of an inverse design workflow that leverages the novel ANN-based ROM method
- Application of the inverse design methodology to numerical optimization of electrically-driven active metasurfaces
- Scientific publications

Skills

Technical skills and level required

- Sound knowledge of numerical analysis for PDEs
- Sound knowledge of Machine Learning / Deep Learning with Artificial Neural Networks
- Basic knowledge of physiscs of electromagnetic wave propagation

Software development skills : Python and Fortran 2003, parallel programming with MPI and OpenMP

Relational skills : team worker (verbal communication, active listening, motivation and commitment)

Other valued appreciated : good level of spoken and written english

EU citizenship is mandatory

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 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
- Contribution to mutual insurance (subject to conditions)

Remuneration

Gross Salary per month: 2100€ gross per month (year 1 & 2) and 2190€ gross per month (year 3)

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 :** 2024-04-01
- **Duration of contract :** 3 years
- **Deadline to apply :** 2024-12-31

Contacts

- **Inria Team :** ATLANTIS
- **PhD Supervisor :**
  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.