

# Offer #2023-07051

# Internship position F/M Reduced-order modeling with Artificial Neural Networks for nanophotonics

Contract type: Internship agreement

Level of qualifications required: Graduate degree or equivalent

Other valued qualifications: Master in applied mathematics or scientific computing

Fonction: Internship Research

## 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

Nanophotonics is the science that studies the interactions between light and matter at the nanoscale. Light is an electromagnetic wave whose wavelength is in the visible spectrum, i.e., between approximately 400 nm to 800 nm. In this context, one refers to as sub-wavelength structuring of matter. The structuring of matter at these scales allows these interactions to be shaped for a variety of technological and societal applications. Among the technological applications of nanophotonics are the control of solar energy (nanostructured solar cells for photovoltaic panels, or for photovoltaic devices embedded in intelligent), improving the sensitivity of digital imagers (nanostructured CMOS image sensors for smartphones, tablets and digital cameras), improving the extraction and emission of light in optoelectronic devices (microLED-based displays). Societal applications are in particular concerned with human well-being (nanoparticle-based therapeutic strategies, biosensing for the detection of viruses). Numerical modeling is extensively used for understanding the physical phenomena underlying lightmatter interactions, but also for tailoring or harnessing these interactions guided by specific performance objectives. The first objective requires to numerically solve the system of time-domain or frequency-domain Maxwell equations coupled to differential equations modeling the behavior of propagation media at optical frequencies while teh seond goal is addressed by leveraghing a numerical optimization algorithm in the framework of an inverse design workflow. For both objectives, the Atlantis team is developing the DIOGENeS [https://diogenes.inria.fr/] software suite, which is dedicated to the numerical study of multiscale problems relevant tonanophotonics and nanoplasmonics. DIOGENeS implements several Discontinuous Galerkin (DG) type methods for which the team has developed a longterm expertise [1-3]. It also includes a includes an inverse design component, which relies on statistical learning-based global optimization methods for single-objectove, multi-objective and robust optimization [4-6].

Beside the above-mentioned high-fidelity DG-based electromagnetic solvers, the team is 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 (Discontinuous Galerkin Time-Domain) electromagnetic solver [1-2]. 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 [7].

[1] 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, Dec 2015.

[2] 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., Vol. 39, No. 3, pp. A831–A859 (2017)

[3] E. Agullo, L. Giraud, A. Gobé, M. Kuhn, S. Lanteri and L. Moya. *High order HDG method and domain decomposition solvers for frequency II domain electromagnetics*. Int. J. Numer. Model. Electr. Netw. Dev. Fields, Vol. 33, No. 2 (2019)

[4] M.M.R. 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)

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

[6] M.M.R. Elsawy, M. Binois, R. Duvigneau, S. Lanteri and P. Genevet. Optimization of metasurfaces under geometrical uncertainty using statistical learning. Optics Express, Vol. 29, pp. 29887-29898 (2021)

[7] K. Li, T.-Z. Huang, L. Li and S. Lanteri. Non-intrusive reduced-order modeling of parameterized electromagnetic scattering problems using cubic spline interpolation. J. Sci. Comp., Vol. 87, Art. no. 52 (2021)

# **Assignment**

Although the non-intrusive POD-based ROM method introduced in[7] 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) [8-10]. In the present internship project, we propose to investigate such an approach for the particular modeling context of nanophotonics.

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

[9] 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)

[10] 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)

This internship work is expected to be a first step toward a PhD project that will be concerned with the development of an advanced computational design methodology for studying and improving the performance of CMOS imagers. This PhD project will be funded a Cifre grant in the framework of a collaboration between the Atlantis project-team of Inria research center at Université Côte d'Azur and STMicrolectronics (CMOS Imagers division of the Technology for Optical Sensors department) in Crolles. Starting from the achievements during the intership, the PhD work will aim at three main objectives: (1) the development of an ANN-based non-intrusive ROM methodology for threedimensional parameterized time-domain electromagnetic problems able to deal with parametrized geometrical features; (2) the development of single-objective and multi-objective inverse design strategies that leverage the ANN-based non-intrusive ROM methodology; (3) the application of the methodology resulting from (1)-(2) to the design of CMOS imagers.

#### Main activities

- Bibliography study on existing ANN-based ROM methods
- Formulation of an ANN-based ROM method for time-domain nanophotonics
- Development (in Fortran 2003 and Python) of the ANN-based ROM method for 3d problems
  Detailed assessment of the novel ANN-based ROM method by considering model problems
- Scientific publication

### Skills

Technical skills and level required:

- Master or engineering degree in numerical mathematics or scientific computing
- Sound knowledge of numerical analysis for PDEs
- Basic knowledge of physiscs of electromagnetic wave propagation

Software development skills: Python and Fortran 2003

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

Other valued appreciated: good level of spoken and written english

#### **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: 2024-03-01 • Duration of contract: 6 months • Deadline to apply: 2024-12-31

#### Contacts

Inria Team : ATLANTIS

 Recruiter: Lanteri Stéphane / <u>Stephane.Lanteri@inria.fr</u>

## **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.