

# Offer #2024-07451

# PhD Position F/M Bayesian Inverse Problems for Wave Propagation towards Exascale

Contract type: Fixed-term contract

Level of qualifications required: Graduate degree or equivalent

Fonction: PhD Position

## About the research centre or Inria department

The Inria center at the University of Bordeaux is one of the nine Inria centers in France and has about twenty research teams.. The Inria centre is a major and recognized player in the field of digital sciences. It is at the heart of a rich R&D and innovation ecosystem: highly innovative SMEs, large industrial groups, competitiveness clusters, research and higher education players, laboratories of excellence, technological research institute...

#### Context

In the framework of the ExaMA project within the NumPEx program (https://numpex.irisa.fr/), we propose a PhD thesis on the topic of Ensemble and Machine Learning Methods for Bayesian Inverse Problems. The

objective of NumPEx is to develop an exascale software stack, and the Exa-MA project is dedicated to the mathematical algorithms to achieve this. The Inria MAKUTU project specilalizes in inverse problems for wave propagation problems and the theoretical and numerical methods needed for their solution

## **Assignment**

In an inverse problem, we seek the (unknown) model parameters from (known) measurements of the system's solution. The direct system—in our case a partial differential equation with its boundary and initial conditions—

can be considered as an operator from parameter space into data/observation space. The inverse problem, from data space into parameter space, is ill-posed [1, 2]. The deterministic approach for solving the inverse problem consists of

minimizing a cost function that expresses the error, or mismatch, between the model predictions and the measured observations, or data. We usually add a regularization term (Tikhonov approach) to penalize solutions that are too os-

cillatory. This nonlinear minimization is usually performed by a method from the quasi-Newton family [3].

Bayes' Theorem provides a framework for the solution of a more general inverse problem, where we seek the posterior probability distribution of a function, given prior knowledge of its distribution and measurements of an observed quantity that depends on the unknown, or hidden function. Mathematically, the theorem quantifies a posterior probability distribution (ppd) as a function of an a priori distribution that captures any previous knowledge about the parameters, and a likelihood function that is obtained by solving the direct model for given parameter values. The resulting a posteriori law is both the solution of the inverse problem and provides a complete quantification of the uncertainty in this solution. The posterior distribution is usually simulated using Markov Chain Monte Carlo (MCMC) methods [2,4], though in this project we will emply

- ensemble Kalman filters,
- · machine learning.
- [1] M. Asch, M. Bocquet, M. Nodet. Data Assimilation: Methods, Algorithms and Applications. SIAM. 2016.
- [2] M. Asch. A Toolbox for Digital Twins: from Model-Based to Data-Driven. SIAM. 2022.
- [3] J. Nocedal, S. Wright. Numerical Optimization. Springer. 2006.
- [4] A. Gelman, J. Carlin, H. Stern, D. Dunson, A. Vehtari, D. Rubin. Bayesian Data Analysis, 3rd edition. CRC Press, 2014

#### Main activities

In this thesis, we want to study, both theoretically and numerically, the solution of inverse problems for wave propagation. A simple case is described by the acoustic wave equation, in a bounded domain, with varying sound speed function over the domain. This case can by easily generalized to more realistic wave propagation problems, including elastic and anisotropic effects.

1. Based on [5], formulate the Bayesian inverse problem (BIP) for the wave equation.

- 2. Give all details of the existence, and convergence properites of the BIP solution.
  3. Propose a MCMC method [2, 4] for solving the BIP. An alternative approach for solving the BIP, is to use an ensemble Kalman filter (EnKF) [1, 2]. This method is known as ensemble Kalman inversion, and was first formulated in [6].
- 4. Based on [6], formulate the EKI approach for the wave equation.
- 5. Give all details of the existence, and convergence properites of the EKI solution.
- 6. Propose a EnKF method [2] for solving the EKI problem.

In a second phase, we will consider machine learning based surrogates that can be used to replace the very costly evaluation of the direct propagation model, especially in 3D space. The machine learning model will be based on a PINN approach [7]. Both MCMC and EKI are methods that can be readily parallelized. This is the ultimate goal of the ExaMA project: to develop a highly parallelized library for the solution of inverse problems in wave propagation. In a final phase, we will then consider scaling up to very large inverse problems on Exascale-ready computing platforms. For this we will generalize the MELISSA-DA framework [8] to the solution of a wide class of inverse problems for wave propagation. This part of the thesis will be done in close collaboration with the DataMove INRIA team https://www.inria.fr/en/datamove.

- [1] M. Asch, M. Bocquet, M. Nodet. Data Assimilation: Methods, Algorithms and Applications. SIAM. 2016.
- [2] M. Asch. A Toolbox for Digital Twins: from Model-Based to Data-Driven. SIAM. 2022.
- [4] A. Gelman, J. Carlin, H. Stern, D. Dunson, A. Vehtari, D. Rubin. Bayesian Data Analysis, 3rd edition. CRC Press, 2014
- [5] A. Stuart. (2010). Inverse problems: A Bayesian perspective. Acta Numerica, 19, 451-559. doi:10.1017/S0962492910000061.
- [6] M. A. Iglesias, K. J. H. Law and A. M. Stuart. Ensemble Kalman methods for inverse problems. Inverse Problems 29 (2013).
- [7] M. Raissi, P. Perdikaris, and G.E. Karniadakis. Physics-Informed Neural Networks: A Deep Learning Framework for Solving Forward and Inverse Problems Involving Nonlinear Partial Differential Equations. Journal of Computational Physics, Volume 378, 1 February 2019, Pages 686-707. https://doi.org/10.1016/j.jcp.2018.10.045
- [8] Friedemann S, Raffin B. An elastic framework for ensemble-based large-scale data assimilation. The International Journal of High Performance Computing Applications. 2022;36(4):543-563. doi:10.1177/10943420221110507

#### Skills

Technical skills and level required: skills in applied mathematics for partial differential equations as well as knowledge of probability and stochastic differential equations; numerical skills and coding experience

Languages: english

# **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 partial 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
- Social security coverage

#### Remuneration

- 2100€ / month (before taxes) during the first 2 years,
  2190€ / month (before taxes) during the third year.

#### **General Information**

- Theme/Domain: Numerical schemes and simulations Scientific computing (BAP E)
- Town/city: Pau
- Inria Center : Centre Inria de l'université de Bordeaux
- Starting date:2024-10-01
  Duration of contract:3 years
  Deadline to apply:2024-05-29

#### **Contacts**

Inria Team : MAKUTUPhD Supervisor :

Barucq Helene / Helene.Barucq@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.

## The keys to success

The candidate should have strong skills in applied mathematics for partial differential equations as well as knowledge of probability and stochastic differential equations. The thesis also requires numerical skills and coding experience to solve the underlying partial differential equations and to implement the stochastic simulation methods. Basic knowledge of machine learning will be appreciated. The candidate should be at ease in English, including reading, understanding and communication.

The thesis will be co-supervised by Prof. Mark Asch, who has a long experience in data assimilation and inverse problems.

Most of the work will take place in Pau, on the office of the Makutu team hosted by the Université de Pau et des Pays de l'Adour. Missions to Grenoble will be organized to foster collaboration with the Inria Datamove team. The doctoral student will have the opportunity to follow training courses that may help him/her to successfully complete his/her thesis project. She/he will be encouraged to take part in conferences to present their results, and to write publications in peer-reviewed journals.

**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

Thank you to send:

- CV
- Cover letter
- Master marks and ranking
- Support letter(s)

#### 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.