General Public Summary

Most mathematical models of natural phenomena are grounded in an understanding of biological and physical processes, allowing us to propose a general structure for the equations. The subsequent step involves validating and calibrating the model using empirical data, a task that often presents significant scientific challenges. Despite being crucial for the model's predictive accuracy, this step is seldom pursued. This project aims to address these challenges by establishing the necessary analytical framework, with a focus on parameter identification for models of various processes, such as tumour growth, traffic flow, and geophysical phenomena. A key strength of the project lies in its innovative application and development of partial differential equation (PDE) techniques, seamlessly integrated with statistical methods. This robust combination drives substantial advancements in optimization, sampling, inference, and machine learning. On one side, statistical approaches such as Bayesian inference play a critical role in identifying the parameters of PDEs, while on the other, newly emerging gradient flow methods hold significant potential for the development of sampling algorithms. The research goals are structured into the following primary tasks:

Parameter identification: The problem of parameter identification is a critical step towards developing truly applicable models. Theoretical analysis of nonlinear PDEs, an area of ongoing research, addresses many complex issues, such as the existence, uniqueness, and regularity of solutions. However, to advance to the next stages—building numerical algorithms, conducting computations, and predicting real-world processes—the calibration of certain equation parameters becomes essential. When these parameters are not known a priori, there are various methods available to determine them.

Sampling methods: Sampling involves selecting representative data points from a larger dataset to estimate the characteristics of the entire population. This problem, especially when dealing with a probability distribution known only up to a normalization constant, is fundamental in computational science, engineering, and Bayesian statistics. Recent research suggests that gradient flow-based algorithms in the space of probability measures offer new directions for sampling. We aim to advance this field, tailoring gradient flow specifications to develop precise algorithms, which are crucial not only for sampling but also for parameter identification.

Stability on parameters: The project aims to advance the understanding and development of new analytical methods for studying how solutions to strongly nonlinear partial differential equations (PDEs) depend on parameters. Despite their relevance, issues concerning the dependence of solutions on parameters, such as Hölder (or Lipschitz) continuity and differentiability, remain largely unexplored. Notably, the stability of solutions with respect to parameters is crucial for validating and calibrating models in biomedical and engineering contexts, as well as in optimization problems where control equations are sought to minimize a functional. A key challenge lies in determining the regularity of solutions relative to parameters. For practical applications, choosing numerical methods with optimal convergence rates should align with the expected solution regularity. Such an approach will allow us to distinguish between numerical methods that are purely heuristic from those whose correctness, including the rate of convergence, can be rigorously established.

Extended graphons: A significant challenge in the project lies in deriving the mean-field limit for multi-agent systems on a wide range of sparse graphs, known as extended graphons. This is particularly focused on non-exchangeable multi-agent systems with non-identical agents. The analysis draws on various disciplines, including partial differential equations, stochastic analysis, and graph theory. The novel concept of limits for extended graphons captures the network's connectivity structure, which plays a crucial role in collective dynamics. Although this area has seen considerable research activity, it has so far been confined to conservative systems. The project's goal is to extend this concept to non-conservative systems, which is highly significant given that most biological models are expressed as balance laws rather than conservation laws.