



# PHD COURSE IN MATHEMATICAL MODELS AND METHODS IN ENGINEERING

Chair:  
Prof. Michele Correggi

Mathematics is everywhere, represented by equations. Between the atmosphere and the wing of a spaceship, in the blood flowing in an artery, on the demarcation line between ice and water at the poles, in the motion of the tides, in the charge density of a semiconductor, in the compression algorithms of a signal sending images from outer space. The equations represent real problems. The Mathematical Engineer can see and understand the nature of these equations, and can develop models in order to understand their relevant qualities and solve real problems. This PhD program aims at training young researchers by providing them with a strong mathematical background and with ability to apply their knowledge to the solution of real-world problems that arise in various areas of science, technology, industry, finance, management, whenever advanced methods are required in analysis, design, planning, decision and control activities. PhD students carry out their research both in the development of new mathematical methods and in the implementation and improvement of advanced techniques in connection with specific contexts and applications.

The Faculty of the PhD program is responsible for the organization of the training and research activities of the PhD students. Decisions of the Faculty comply with the requirements and standards of the Doctoral School of the Politecnico di Milano. A Chairman is elected within the Faculty, for representative and coordination activities. Admission of students to the PhD program is decided after examination of the candidates. Students applying to our program must provide their CV, along with reference and motivation letters. After admission, each student is assigned a tutor. The tutor is a member of the Faculty who assists the student in the early stages of his career, especially in the choice of the courses and in identifying a thesis advisor.

The PhD program has a duration of three years. Activities include: soft skills courses; specialized courses; research training, including seminars, tutoring activity, participation to workshops/conferences, and scientific publications; development of a doctoral thesis.

At the end of each academic year, the PhD students report to the Faculty about their activity. The students report about attendance of courses and exams (and the corresponding grades), participation in various scientific

activities (seminars, conferences, summer schools etc.), planning and intermediate results on their research project and preparation of the PhD thesis, and any other relevant activity. At the annual meeting the students also receive a grade by the Faculty. A negative grade may entail repetition of the current year of doctoral study (with suspension of the grant, if any) or exclusion from the PhD program, depending on the Faculty's decision. Mobility of PhD students to other institutions is strongly encouraged and financial support is provided to this purpose.

Among others, let us mention some typical types of professional skills and possible occupations of the graduated Doctors: analytic and numerical treatment of differential models for physical and industrial problems, quantitative methods in finance and risk management, operations research and optimisation, statistical modelling and data analysis.

Placement of graduated Doctors is expected in the following positions: research and development divisions of businesses, businesses involved in innovative design activities, financial institutions such as banks or insurance companies, public or private research centres, public and/or governmental agencies for social, economical, scientific study, planning or evaluation, Universities.

Since the PhD program in Mathematical Models and Methods in Engineering (formerly, Mathematical Engineering) has been active since the year 2001, we expect that a larger number of institutions and businesses will soon become more and more aware of the professional skills and expertise of graduated doctors.

**Grants funded by external partners:** IIT, Leonardo Spa, Pirelli Tyre Spa, ENI Spa, RSE, Intellico

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# PRIVACY-PRESERVING DATA ANALYSIS OF LOCATION DATA FOR THE DESIGN OF HUMAN MOBILITY SERVICES AND INFRASTRUCTURES

Arianna Burzacchi – Supervisor: Simone Vantini

Thanks to the technological revolution, we are witnessing the creation of large databases of new high-resolution mobility information. The usefulness of their applications is undeniable and spans a wide range of research fields, from the study of human mobility to health, environmental, and social studies. Along with the new interest in these data, however, comes the need to limit the risk of sensitive information disclosure. Indeed, basic Statistical Disclosure Control (SDC) methods are not always sufficient to fully mask the identities of individuals within the data. A significant effort has been made by the governments to propose and enact comprehensive consumer privacy legislation. Up to now, 80% of the countries worldwide has, or is planning to, put in place legislation to secure the protection of data and privacy. All of these legislations serve as guarantees that there is at least a lower bound for privacy disclosure risk to be respected, ensuring the security of the original data owners. In light of this, new innovative approaches are needed to properly balance the utility and the privacy of the data, enabling the leveraging of the overall information captured in datasets while ensuring that

sensitive information of individual persons remains protected and private. This Ph.D. thesis raises in this framework seeking to improve the potential of mobility data availability while focusing the attention on the sensitivity of the information of the underlying individuals. The aim is to find the optimal ways to exploit mobility data in a privacy-compliant form, developing novel pipelines and statistical methodologies to properly understand, analyze, and model mobility data. Specifically, mobility data is the starting point of three analyses, characterized by distinct practical motivations, input data type, and theoretical data modeling, but with the common intention of leveraging the mobility data in the most efficient and useful way in strict adherence to privacy principles. The first analysis focuses on mobility services and evaluates the efficiency and the efficacy of the urban public transportation system in Milan, Italy. The research questions tackled in the study are *How can we monitor and analyze the public surface transportation system? Which is the criticality of the current mobility service offered? And how can it be addressed?* Hence, the main motivation of the study is the analysis of mobility data

towards supporting and guiding public transport operators in maximizing the balance between the mobility demand and the offered service. Beyond this goal, the study aims at the construction of a pipeline to systematically analyze the quality and reliability of the available data. While addressing these tasks, the main source of information is the Automatic Passenger Counting (APC) sensor data recording the number of passengers boarding, alighting, and on-board of a pilot route in the surface network. Due to the inherent anonymization of APC measures, the analysis is carried out without significant privacy concerns. The main challenge is however to extract meaningful information from counting data, making the most of the spatial and temporal granularity of the data. From the methodological point of view, the research is aimed at finding the right model for this data characterized by variability in time and in space. After modeling its grouping structure inherited by the stops, a comparison of statistical methods (Generalized Linear Mixed-effect Models, GLMMs) and machine learning methods (Generalized Mixed-Effect Random Forests, GMERFs) is conducted. By applying such advanced models to study

mobility data, for the first time, the research highlights both their limitations and usefulness while addressing the research questions. Then, the naturally anonymized input data is substituted with the use of user specific data. The main data source of the remaining analyses is Global Positioning System (GPS) traces from users' smartphones. In the second analysis of the thesis, in order to mitigate the risks of privacy disclosure and ensure compliance with data protection standards, the original microdata is subject to a rigorous process of aggregation and combination. By aggregating the data, the detailed individual-specific trajectories are transformed into broader patterns that represent collective mobility trends rather than isolating the actions of any user. Specifically, the original GPS measures are leveraged to obtain accessibility maps of points of interest, where each point in the map is associated with an accessibility measure, i.e., the travel time to the point of interest. Accessibility maps do not pose a privacy issue because they aggregate GPS data to show generalized travel times to points of interest, focusing on spatial accessibility rather than individual movements or personal information. The focus of the research is specifically on the accessibility of university institutions applied to the case study of Politecnico di Milano, providing useful heatmaps to describe the travel time variation as a measure of accessibility around the metropolitan area.

The analysis then moves its attention forward and focuses on the impact of accessibility on the academic performances of university students. The main research question is indeed *How does the travel time to university impact the students' grades?*, utilizing the travel time as a measure for accessibility and the Grade Point Average (GPA) for academic performances. The answer is provided by an innovative two-step process of data analysis made of advanced statistical and machine learning methods from Kernel Regression to causal inference. In contrast to the data aggregation, the third and last analysis describes another solution to the privacy attack risk of non-aggregated user specific mobility data. A new analytical pipeline is introduced to generate synthetic data, which is similar enough to the original one to capture its valuable information, while different enough from the original data not to be associated with any specific individual. Synthetic data generation (SDG) methodologies are spreading in the world of statistical database privacy because provide ways to anonymize large databases without the use of SDC techniques, hence allowing application to complex structures of data. The proposed SDG method is built and applied to GPS trajectories. In the study case, trajectories are recorded in the Milan metropolitan area and share a common terminus in a point of interest. These are modeled as three-dimensional functions in an optimal mathematical space, with

coordinates and elapsed-time varying on the trip completion percentage, framing the analysis in the context of Functional Data Analysis and Shape Analysis. The generation process follows an object-oriented statistical approach for which, for each original function, a synthetic twin is computed by means of the averaging of its neighbors with stochastic weights. The research goal is hence to synthesize new datasets of GPS trajectories. However, given the flexibility of the proposed modeling and analytical framework, the application of the method is straightforward to any functional data and hence answers the more general question of how to synthesize new functional datasets. Moreover, emphasis is placed on the evaluation framework for the SDG method, assessing the quality of the synthetic data through the analysis of representative measures for privacy and utility. This research investigates the extent to which synthetic data mimics the original one while ensuring the privacy compliance of the technique.

# ENHANCING NUMERICAL METHODS THROUGH DEEP LEARNING

Matteo Caldana – Supervisor: Paola F. Antonietti

Co-Supervisor: Luca Dedè

Deep learning has rapidly emerged as a powerful tool across various applied science and engineering domains. This thesis explores the field of scientific machine learning (SciML) which stands at the intersection between deep learning and numerical methods, focusing on enhancing the efficiency of numerical algorithms through innovative developments and applications of deep learning. The thesis addresses three novel developments in the field of scientific machine learning, all designed to improve the efficiency of numerical methods while enhancing their stability and reducing computational complexity. In the first part of this thesis, we propose a deep learning-based algorithm to optimize the efficiency of Algebraic Multigrid (AMG) methods, a state-of-the-art solver for large linear systems stemming from the discretization of partial differential equations (PDEs). We propose a deep learning-based algorithm that is able to automatically tune on-the-flight the strong threshold parameter in AMG to minimize the computational time needed to solve the linear system at hand. The main difference with the previous works is that our algorithm is completely

non-intrusive: it does not require any change to existing code (neither to the FEM nor the AMG solver). This guarantees a wider range of applicability and means that we can rely on all the classical theoretical results regarding convergence. The neural network (NN) leverages an ad-hoc defined pooling operator and a convolutional neural network (CNN) to extract the relevant features from the sparse matrix of the system. The NN-enhanced AMG method reduces significantly the computational cost, that is the elapsed time, (see Fig. 1) needed to solve the linear system compared to employing the pre-defined choice of the parameters based on trial-and-error, experience, and literature. The second part of the thesis addresses the challenge of handling oscillations in the numerical discretization of hyperbolic PDEs with high-order methods. Indeed, near discontinuities, high-order solvers face challenges due to the Gibbs phenomenon. We introduce a novel artificial viscosity model, trained using a hybrid learning approach that combines reinforcement learning with physics-informed machine learning. Namely, thanks to automatic differentiation, we can differentiate through the

RL environment, effectively embedding information on the physics of the problem into the learning dynamics. This method dynamically adjusts the viscosity in response to solution irregularities, thereby preserving stability and accuracy without the need for problem-specific parameter tuning. This also enables seamless integration of noisy data obtained from measurements of quantities of interest into the loss function, thereby being able to learn new physical models directly from data. The approach is validated on a range of hyperbolic PDEs – including Burger's and Euler's equations and the KPP rotating wave (see Fig.2) – showcasing its ability to accurately detect spurious oscillations and tune suitable artificial viscosity while maintaining physical consistency.

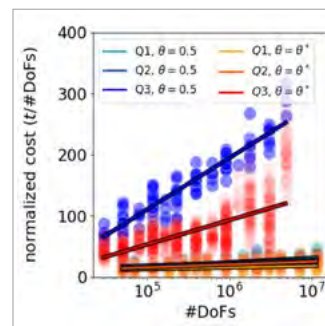


Fig. 1 - Comparison of the computational cost of the classic AMG (blue) and the NN-enhanced AMG (red)

Finally, we tackle the issue of stiffness in reduced-order models (ROMs) using neural ordinary differential equations (ODEs). Stiffness, characterized by rapid changes in certain solution components, poses significant numerical challenges because it requires prohibitively small time steps for explicit solvers. Our approach employs a neural ODE to learn a time-reparametrized

stiff system, where the time map is suitably built so to reduce the stiffness of the problem. The insight is to introduce a data-driven time reparametrization of an implicit solver as a way to reduce the stiffness of the system. Thus, it is possible to solve the neural ODE with an explicit solver, thereby enhancing the efficiency and stability of

the neural ODE architecture. We validate our method through extensive experiments on relevant problems used in the literature to benchmark stiff solvers. In Fig. 3 we show an example of the predictions made on the Oregonator model.

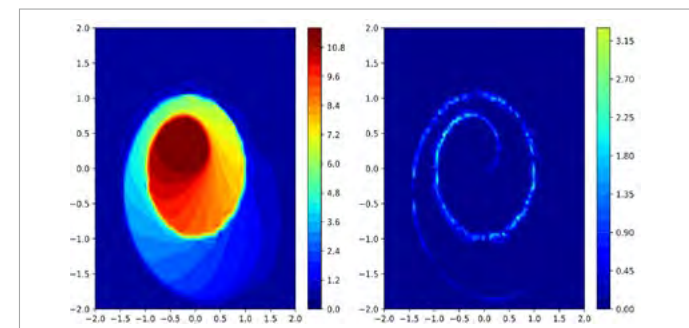


Fig. 2 - The KPP rotating wave stabilized with the neural artificial viscosity (left) and the error with respect to the reference solution (right)

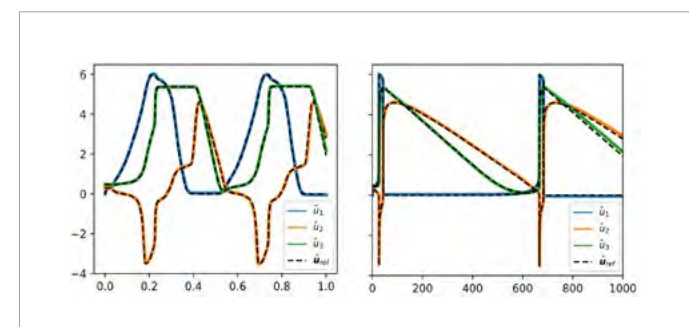


Fig. 3 - Prediction of the neural ODE on the Oregonator model in the reparametrized time (left) and the prediction mapped to the original time (right)

# MATHEMATICAL MODELS AND NUMERICAL METHODS FOR NEURODEGENERATIVE DISEASES

**Mattia Corti** – Supervisor: Paola F. Antonietti

Neurodegenerative diseases represent a significant societal challenge. Indeed, due to the aging of the global population, the number of people affected by these pathologies is constantly increasing. According to the World Health Organization (WHO), around 50 million people were affected by dementia in 2020. This number is expected to reach 132 million people in 2050. Some neurodegenerative diseases, known as proteinopathies, are characterized by the misfolding of proteins. This misfolding leads to the generation of toxic proteins that spread and aggregate inside the Central Nervous System. Medical research has found evidence that the altered structure of these proteins is linked to resistance to clearance mechanisms, which in turn leads to the aggregation of proteins and the death of neurons. However, there is a significant delay between protein misfolding and the appearance of clinical symptoms, often spanning decades. This unbalanced progression of the disease complicates the development of efficient medical treatments. Diseases such as Alzheimer's, Parkinson's, Amyotrophic Lateral Sclerosis (ALS), and Lewy body dementia follow this pattern,

with specific proteins showing stereotypical progression. To better highlight the differences between all these pathologies (often co-existing), in recent years, several mathematical models for the dynamics of prion-like proteins have been proposed. A mathematical description of the spreading of these proteins is of primary importance in providing valuable insights into the disease progression. At the same time, some numerical methods have been developed to simulate in-silico phenomena. However, the geometric complexity of the brain requires the design of advanced numerical methods to approximate the models. The goal of this thesis is threefold: to construct efficient numerical schemes for the simulation of neurodegenerative diseases, to derive a systematic way to estimate the model parameters towards personalized models, and to propose open-source scientific computing tools accelerated with machine learning techniques. First, we want to construct efficient and accurate numerical methods for simulating neurodegenerative disease phenomena in real brain geometries. In this context, the quality of a numerical method is connected to preserving features of the brain sulci and

substructures with a reasonable number of degrees of freedom. The achievement of this goal requires polytopal mesh grids and high-order numerical methods. Moreover, positivity-preserving numerical schemes need to be discussed to preserve the physical meaning of the numerical solution in simulations of protein spreading (Fig. 1) and maintain the efficiency of the numerical solver. To construct patient-specific numerical simulations of prion-like spreading associated with different pathologies, we need to design some calibration techniques for the physical parameters of the Partial Differential Equations. In particular, the calibration can be based on protein concentrations derived from medical images, such as Positron Emission Tomography. For this purpose, we

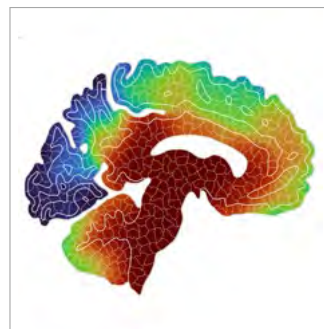


Fig. 1 - Alpha-synuclein spreading simulation in Parkinson's disease

need to adopt inverse Uncertainty Quantification methods coupled with reduced-order numerical discretization methods (Fig 2). Another possibility is calibrating the parameters starting from biological post-mortem measurements in the brain cortex. These calibrations are related to the limits of applicability of the different mathematical models that need to be analyzed to validate the clinical meaning of the results. Finally, detailed numerical simulations require enhanced techniques to construct polytopal mesh grids and polytopal method solvers. Agglomeration techniques should be able to preserve a detailed

description of brain interfaces (cortex boundaries or white-grey matter interface). Graph Neural Network techniques allow the automatic treatment of physical parameters within the agglomeration procedure. Designing open-source libraries to simulate multiphysics systems through polytopal methods is a fundamental step in validating the efficiency of our techniques. This thesis introduces lymph (discontinuous poLYtopal methods for Multi-PHysics), an open-source MATLAB library for the PolyDG approximation of multi-physics problems in two dimensions (Fig. 3).

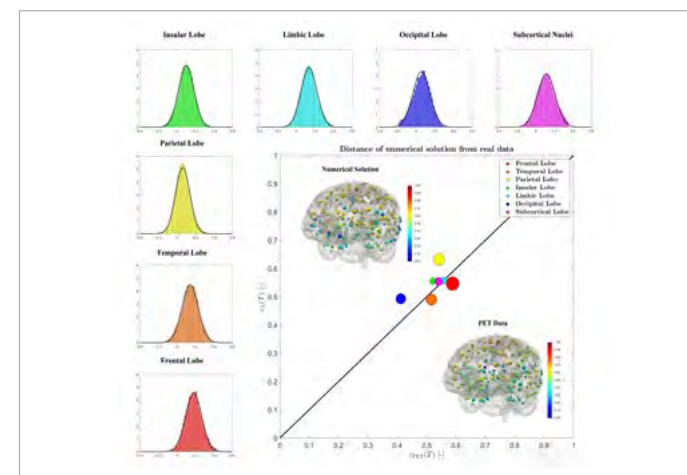


Fig. 2 - Fisher-Kolmogorov reaction parameter distributions in Alzheimer's disease

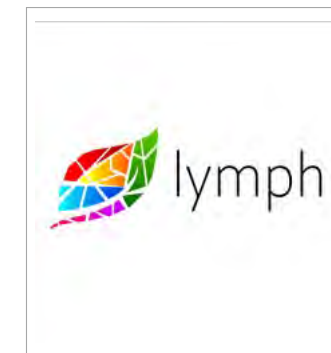


Fig. 3 - Lymph library logo

# PARTICLE-BASED NUMERICAL METHODS FOR LANDSLIDES: RUN-OUT AND IMPACT ANALYSIS

**Marco Fois** - Supervisor: Luca Formaggia

Co-Supervisors: Carlo De Falco, Simona Perotto

This doctoral thesis addresses the issue of climate change and the associated hydrogeological risks, with a particular focus on landslide phenomena such as mudflows and debris falls. These events pose significant threats to both infrastructure and the environment, making it crucial to develop advanced modeling techniques that can accurately predict their behavior. The main objective of this research is the development of innovative numerical models, with a specific emphasis on particle-based methods, for the simulation of such events. The study focuses on both the runout phase, where the material propagates along the terrain, and the impact phase, where the landslide interacts with protective structures.

A key aspect of this work is the implementation of a two-step variant of the second-order explicit Taylor-Galerkin method (TG2). This finite element-based scheme has been enhanced with a Lagrangian front-tracking technique and a flux limiter, which significantly improve its accuracy and stability in capturing rapid and complex material deformations. Additionally, the method has been made adaptive in both time and space, allowing it to dynamically adjust the computational

resolution based on the evolving characteristics of the landslide. The developed numerical code was subsequently parallelized to ensure computational efficiency and was tested on a wide range of benchmarks and real-world case studies, demonstrating its robustness and applicability. Parallel to this, different discretization techniques based on particle-based approaches were explored and refined to improve the handling of large deformations, which traditional mesh-based methods often struggle with. These methods also allow for a more detailed treatment of the impact phase against barriers and structures, which is crucial for evaluating the forces and stresses exerted by the landslide on built environments. In particular, a semi-conservative variant of the Material Point Method (MPM) was developed and implemented. This method, derived from the Particle-in-Cell (PIC) approach formulated in the mid-1990s, offers a powerful framework for modeling highly dynamic and large-deformation problems. Originally designed for continuum mechanics analysis, this approach was coherently adapted to the depth-averaged model used in this study, known as the Depth-Averaged MPM

(DAMPM). The adaptation involved incorporating essential physical factors such as the hydrostatic pressure gradient, topography, and rheology, ensuring that the model could accurately capture the behavior of real landslide events. The developed code underwent extensive validation through benchmarks featuring both simple and complex topologies and was successfully applied to several real-world case studies, reinforcing its practical relevance.

The second part of the thesis focuses on the crucial challenge of analyzing the impact phase, where landslides interact with protective barriers and other structures. This is approached using a multiscale modeling framework that effectively integrates two-dimensional and three-dimensional simulations. Specifically, the DAMPM solver

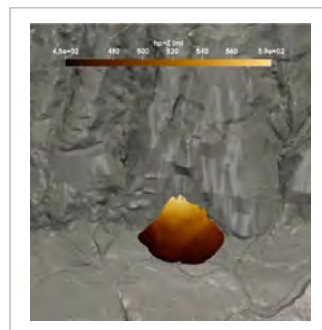


Fig. 1 - Bindo-CortenoVA landslide

developed for runout simulations was coupled with a 3D MPM model to leverage the computational efficiency of 2D simulations in the early stages of the landslide while transitioning to a more detailed 3D representation in the later impact phase.

To ensure consistency between these different modeling scales, a dedicated algorithm was developed to transfer information from 2D to 3D while preserving mass and momentum. This step was crucial to maintaining the physical reliability and accuracy of the simulations, allowing for a seamless transition between the different stages of analysis. The work was conducted in collaboration with the research group from the Department of Statics at TUM in Munich, bringing together expertise from multiple disciplines to refine the modeling techniques.

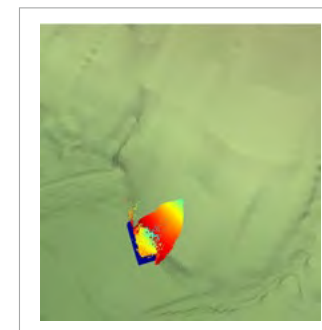


Fig. 2 - Impact of a mudflow on a rigid barrier

Once the coupled model was fully developed, it was rigorously tested on several numerical benchmarks to validate its accuracy and predictive capabilities. Finally, the methodology was applied to a real-world case study, further demonstrating its effectiveness in practical risk assessment scenarios. The results obtained highlight the model's ability to provide valuable insights into the dynamics of landslides, particularly in terms of their trajectory, velocity, and the forces they exert on infrastructure. Overall, this doctoral research introduces new numerical techniques for predicting the behavior of moving masses, taking into account diverse geological and topological conditions. By integrating advanced computational approaches with robust validation strategies, this study contributes to improving risk prevention capabilities and management strategies in the field of hydrogeological hazards. With regard to the impact phase, the thesis presents a novel yet computationally efficient approach for evaluating the energy and force distribution exerted by landslides on infrastructures and the surrounding environment.

The techniques developed in this work allow for rapid analysis while optimizing computational resources, making them particularly suitable for large-scale risk assessment applications. By bridging the gap between high-fidelity simulations and practical implementation, this research provides valuable tools for engineers and policymakers working on landslide mitigation and disaster prevention.

# NUMERICAL METHODS FOR SIMULATION AND OPTIMIZATION OF WAVE ENERGY CONVERTER ARRAYS

**Marco Gambarini** – Supervisor: Edie Miglio

Co-Supervisor: Gabriele Ciaramella

The mitigation of climate change requires the increasing adoption of renewable energy sources. Since their production is influenced by weather events and can thus be only partially scheduled, it is essential to diversify their mix. In this context, marine renewable energies are a significant opportunity, as indicated by their inclusion in the energy strategies of the European Union. This thesis focuses on wave energy extraction devices, known as WECs (Wave Energy Converters), and in particular on arrays of these converters. The need to design large arrays stems from the fact that the typical nominal power output range of WECs is smaller compared to alternative technologies, such as wind turbines. The devices in a park interact with each other through diffraction and radiation processes, whose result is known as the park effect. This can lead to a reduction of the extracted power, if not properly accounted for at the design stage.

In this thesis, we propose mathematical models and numerical methods for the simulation and optimization of WEC parks, which can be useful tools for analysis and preliminary design.

Our first contribution concerns park simulation. For the numerical solution of the linear potential model equations, discretized with the BEM (Boundary Element Method), we introduce a novel preconditioner. It is based on the block-Jacobi method combined with a coarse correction, and it is effective in reducing the number of iterations and the computational time. The preconditioner has been implemented on top of the hierarchical matrix engine of an existing open-source BEM code, Capytaine, and it is available on github.

Regarding optimization, the optimal design problem of a WEC park, with the objective of maximizing the average power output subject to the hydrodynamic state equation, to the slamming constraint and to geometric constraints, has been gradually tackled. First, we focused on the optimization of the control parameters at fixed layout, developing an optimization framework that is robust with respect to the operating uncertainties. We have considered uncertainty with respect to the direction of incident waves, treated through two different stochastic optimization approaches:

stochastic gradient descent and sample-average approximation. For sample-average approximation, we have considered the Monte Carlo and Gauss-Legendre quadrature schemes. Moreover, instead of solving the diffraction problem for each value of the wave direction, we have used a reciprocity relation known in the hydrodynamics community as Haskind's relation to compute diffraction forces from the precomputed radiation potentials, thereby significantly reducing the computational time. After that, we examined the problem of layout optimization, with fixed controls. While the most common approaches in the literature are based on metaheuristic algorithms, we have developed a gradient-based method. The possibility of computing the gradient exists thanks to a suitable choice of the hydrodynamic model. The resulting optimization method has been applied to a park of water turbine OWC (Oscillating Water Column) devices with water turbine. This work has been carried out for the offshore WaveSAX device, developed by the company RSE S.p.A (Ricerca sul Sistema Energetico). For this kind of device, a non-linear, lumped-parameter model has

first been developed using mass and momentum balance equations and the turbine's characteristic curve. This model has been used to estimate the power matrix of a single device by optimizing the turbine's rotational speed for each sea state of interest. Then, the model has been linearized in order to reduce its computational cost and make it suitable for optimization. Park optimization has then been performed assigning to all devices the optimal rotational turbine speed for a representative sea state. The park geometries considered are consistent with the prospective combined installation of wind-wave offshore parks. Finally, the combined problem of optimizing positions and control parameters has been tackled. We have adopted a gradient-flow approach, which permits

the treatment of all constraints in a unified manner, and accepts unfeasible initial guesses, since it includes a feasibility restoration term. The developed method can handle non-convex admissible sea areas, thanks to a formulation based on the regularization of indicator functions. The gradient flow equations are discretized with a Runge-Kutta method with adaptive time step, which combines the Euler and Heun (2<sup>nd</sup> order) methods, while the conjugate gradient method is used to compute the flow direction at each time step. In order to avoid the need of setting hyperparameters by the user, which could potentially be a time-consuming trial and error process, we have introduced an adaptive strategy, which automatically determines suitable tolerances for the conjugate gradient and Runge-Kutta solvers.

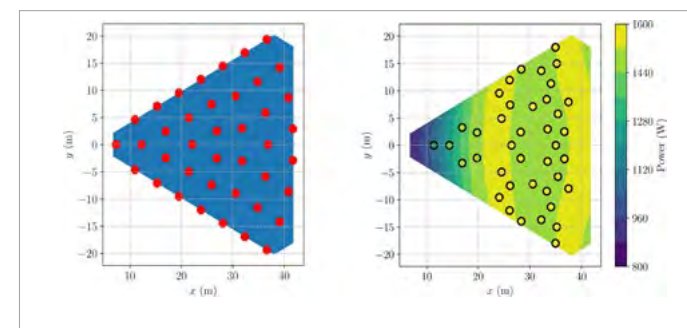


Fig. 1 - Layout optimization of offshore WaveSAX devices: initial guess (left) and optimization result (right).

# BAYESIAN NONPARAMETRIC ANALYSIS OF SPATIAL AND SPATIO-TEMPORAL DATA: MODELLING AND COMPUTATION

**Matteo Gianella** – Supervisor: Alessandra Guglielmi

Spatial and spatio-temporal data, prevalent in fields like environmental science, epidemiology, economics, and urban studies, involve observations tied to specific locations and times. These data are often more similar at closer spatial locations, with temporal changes reflecting evolving patterns. Understanding these interactions is key for addressing real-world issues like disease spread, pollution, and economic disparities.

Advances in data collection, such as satellite imaging and GPS, have made spatial data more available, but also more complex to analyze due to factors like non-linear relationships, spatial heterogeneity, and temporal dependencies. Traditional statistical models struggle with these complexities, and developing flexible models to handle them remains an active research area, with challenges in accounting for varying influences across time and space. New methodologies aim to better capture these intricate patterns and improve predictions and insights from such data.

In this thesis, we adopt a Bayesian approach towards inference. Under this paradigm, the notion of probability is interpreted as the degree of belief of the occurrence of a certain event. The Bayesian

approach also introduces the scientist's prior knowledge about the phenomenon under study into the picture, in the form of suitable probability distributions for parameters, conditionally on which a likelihood for the data is specified. As a consequence, data are used to update this prior belief and provide a more informed knowledge in light of the available observations. In the Bayesian approach, then, the main target is the posterior distribution of such unknown parameters given the data, which can be computed via Bayes' theorem. However, this distribution, in general, is not available in closed form, thus requiring the implementation of suitable Markov Chain Monte Carlo (MCMC) simulation strategies to generate (quasi) i.i.d. samples from this posterior distribution. Under this approach, Bayesian nonparametric models offers flexible models that can capture complex or non-linear dependencies. One of the key advantages of Bayesian nonparametric models is their larger flexibility w.r.t. parametric ones, since they assume an infinite-dimensional parameter space. This makes Bayesian nonparametric methods particularly well-suited to the analysis of spatial and spatio-temporal data, where unknown and

evolving patterns often need to be captured in a flexible manner. However, the analysis of spatial and spatio-temporal data under the Bayesian approach introduces significant challenges also at a computational level, due to the size and complexity of this type of data. Indeed, spatial data typically involve measurements across multiple locations, and spatio-temporal data include variations over time as well, the volume of information can be enormous. Moreover, dependencies between observations (such as spatial correlations or temporal autocorrelations) add further complexity and makes standard MCMC algorithms either inefficient or impractical. Indeed, these algorithms are, in general, computationally intensive for large datasets. This computational burden is only increased in case of spatial data, as at each iteration we require computationally intensive operations to evaluate probability density functions or compute determinants of large matrices. While dealing with complex data as those handled in this dissertation, the design of specialised, efficient and scalable algorithms for posterior inference is crucial.

In this thesis, I have tried to make contributions in the Bayesian analysis of spatial and

spatio-temporal data both on a methodological and computational level. On the methodological point of view, with the help of my supervisor and coauthors of the manuscripts from my thesis' work, I have proposed Bayesian nonparametric models for the analysis of spatial and spatio-temporal data in different scenarios. In particular, I have considered problems such as boundary detection, spatial clustering, and the analysis of high-dimensional datasets. At the same time, a significant effort has been devoted to efficiently design and implement MCMC algorithms for these models. Spatial and spatio-temporal datasets are often large and complex, making it essential to develop efficient algorithms that can handle the scale of the data while providing accurate and meaningful results. To address these computational challenges, this thesis introduces new algorithms for distributed Bayesian inference, as well as efficient and specialized software to facilitate the application of Bayesian nonparametric models to real-world problems. By advancing both the theory and computation of Bayesian nonparametrics, the goal of this work is to make these flexible models more accessible and feasible for applied researchers working with complex spatial and spatio-temporal data. This contribution not only enriches the available Bayesian toolbox for spatial data analysis but hopefully will help bridge the gap between cutting-edge Bayesian statistical theory and applied research in fields where understanding spatial and temporal dynamics is critical.

This doctoral dissertation is composed by 5 chapters and 2 appendices:

- In Chapter 1, I present a Bayesian model for detecting boundaries in spatial data, applied to income distributions in the greater Los Angeles area. The goal is to identify boundaries between areas with significant economic differences, which can help policymakers address inequalities without assuming dissimilarity metrics or available covariates. The model uses a mixture of Gaussian distributions to represent income levels. Posterior inference is attained via a novel trans-dimensional MCMC algorithm that jointly estimate the spatial densities in each area and detect boundaries between areas with different income distributions. Additional details can be found in Appendix A.
- Chapter 2 introduces and extend Consensus Monte Carlo (CMC) algorithms for Bayesian nonparametric clustering in case of large areal datasets. CMC is distributed algorithm for posterior inference designed to handle massive datasets, which cannot be analysed in reasonable time through traditional MCMC methods. The algorithm split the dataset into smaller portions called shards that are fitted in parallel using traditional MCMC algorithms. The "sharded" posterior draws are then combined to produce the so-called consensus posterior. The method is introduced and applied to spatial clustering problems, both in case of continuous and count response variables.
- In Chapter 3 I propose a Bayesian model for clustering spatio-temporal data, with a focus on pollution levels in the Po Valley, Italy. The model helps identify regions where pollution levels change over time and can uncover hidden patterns in the data. I use a product partition model to account for temporal dependencies and apply the model to real-world data, showing how it can be used to detect clusters of high pollution and track their evolution over time.
- Chapter 4 deals with the development of BayesMix, a C++ library that implements MCMC algorithms for the analysis of Bayesian nonparametric mixture models. The library is designed to be modular and flexible and allows users to easily extend its functionality for different applications. After a revision of the available software, I explain the design of BayesMix and provide examples to show its use.
- The final chapter focuses on a side project I finalised during the first year of my PhD programme and deals with spectrometric data. In this case, the goal is to analyse complex relationships between variables using Gaussian graphical models. These models help smooth functional data and learn the underlying structure of high-dimensional datasets. Additional details can be found in Appendix B.

## FOUR ESSAYS IN ENERGY FINANCE

### Pietro Manzoni – Supervisor: Roberto Baviera

In recent years, the field of energy finance has emerged as a prominent area of study, bridging the gap between energy markets and quantitative finance. This discipline addresses the complex challenges of decision-making within the energy sector and energy markets, covering a wide array of activities such as financial management, policymaking, and risk assessment.

This thesis, conducted under the supervision of Professor Roberto Baviera, explores four key frontier challenges in energy finance: probabilistic load forecasting, forecast reliability, stochastic modeling of energy markets, and environmental policy assessment.

i) The first challenge involves developing an advanced forecasting methodology using Recurrent Neural Networks (RNNs), a deep learning technique well-suited for time series forecasting. RNNs are particularly effective in energy forecasting as they capture the sequential dependencies in electricity demand data. We introduce the RNN(p) models, an extension of traditional AutoRegressive models with eXogenous inputs (ARX(p)), which integrate multiple

feedback loops across different time scales. This architecture enables the models to better account for the various factors influencing energy consumption patterns, including seasonal and daily fluctuations.

Our analysis shows that RNN(p) models achieve strong predictive performance in probabilistic load forecasting, effectively capturing uncertainty and variability in energy demand. The high degree of interpretability offered by these models is another key advantage, as it provides insights into the factors influencing energy consumption. By quantifying uncertainty, the RNN(p) models support improved decision-making in energy markets, financial risk management, and policymaking, ultimately enhancing the sector's ability to anticipate demand fluctuations and optimise operational strategies.

ii) The second challenge focuses on the reliability of probabilistic forecasts, ensuring that predicted probabilities accurately represent the actual uncertainties in electricity demand. A key issue in this context is overconfidence, where the model generates forecasts that are too

sharp, underestimating the true variability in the data. Overconfident models pose significant risks in energy finance, potentially leading to flawed risk assessments, financial losses, and grid instability.

To manage overconfidence, we propose a new learning methodology based on modified loss functions specifically designed to correct overly sharp forecasts. These loss functions encourage better uncertainty estimation, thus improving the calibration of probabilistic forecasts. Our empirical analysis of load forecasting data shows that this approach significantly enhances the reliability of predictions, making them more suitable for real-world energy finance applications.

iii) The third challenge focuses on stochastic modelling of energy markets, particularly in the pricing of energy derivatives. Unlike traditional financial markets, energy markets deal with physical commodities such as electricity, which introduces unique constraints like storage limitations and transportation bottlenecks. To model these dynamics, we use Lévy-driven Ornstein-Uhlenbeck (OU)

processes, which effectively capture mean-reverting behavior, irregular price movements, and sudden jumps—key characteristics of energy prices.

A major challenge in applying these models lies in simulating their trajectories efficiently. Existing methods are often computationally intensive and unsuitable for practical use. To address this, we developed a novel simulation algorithm that allows for fast and accurate simulations of Lévy-driven OU processes on a discrete time grid. This method significantly improves the speed and precision of energy price forecasts, enabling more effective pricing of energy derivatives. By enhancing the simulation process, we make it easier to assess market risk and manage price volatility in energy markets.

iv) The fourth and final challenge examines the European Carbon Allowance Market and its role within the European Union Emissions Trading System (EU-ETS), which aims to regulate and reduce greenhouse gas emissions across industries. While the EU-ETS is a key policy tool, it operates on a cap-and-trade system, whereby companies must hold allowances

to emit CO<sub>2</sub>. Unlike other energy markets, the carbon market trades intangible assets – carbon allowances – rather than physical commodities.

We investigate an observed anomaly in the pricing of carbon allowances: a consistent positive spread between the spot/future rate and the actual risk-free rate. Using advanced econometric tools, we analyse the causes of this “carbon spread” and find that it can primarily be explained by credit risk of the companies participating in the scheme. Our work provides robust statistical evidence of the existence of a cointegration relationship between the two quantities, demonstrating that the “carbon spread” is not driven by other financial or commodity factors. Based on these findings, we propose a policy intervention aimed at improving market efficiency and addressing the credit risk component affecting the pricing of carbon allowances.

## THREE ESSAYS ON ESG RATINGS AND QUANTITATIVE FINANCE

**Davide Stocco** – Supervisor: Emilio Barucci

Environmental, Social, and Governance (ESG) scores have become a crucial tool for evaluating corporate sustainability, yet their functioning and their impact on the financial market is still far from being understood. In this thesis, we address three key gaps in the literature. First, we explore the proprietary models used for issuing ESG ratings and their main drivers. Secondly, we examine ESG ratings' role in asset managers' investment decisions. Finally, we analyse the impact of ESG-related controversies and sustainability social media reputation on stock prices. More in details, we first replicate ESG scoring methodology of London Stock Exchange Group (LSEG), former Refinitiv, using machine learning techniques to unveil the key drivers of ESG ratings, with a focus on their balance between forward-looking promises (aspirational) and past achievements (performance). Our analysis demonstrates a high level of consistency of the relevant features over time, with minimal changes as more data become available. Crucially, we find that 60% of the information reflected in ESG scores is based on forward-looking commitments, whereas 40% is derived from past performance. Moreover, we

evaluate several white-box and black-box mathematical models to reconstruct the E, S, and G ratings' assessment model and interpret their main drivers. The results show that it is possible to replicate the underlying issuance process with a satisfying level of accuracy. However, there is evidence of persisting unlearnable noise that even more complex models cannot eliminate. Secondly, we investigate the portfolio frontier and risk premia in equilibrium when an institutional investor aims to minimize the tracking error variance and to attain an ESG score higher than the benchmark's one (ESG mandate). Provided that a negative ESG premium for stocks is priced by the market, we show that an ESG mandate can reduce the mean-variance inefficiency of the portfolio frontier when the asset manager targets a limited over-performance with respect to the benchmark. Instead, for a high over-performance target, an ESG mandate leads to a higher variance. The mean-variance improvement is due to the fact that the ESG mandate induces the asset manager to over-invest in assets with a high mean-standard deviation ratio. In equilibrium, with asset managers and mean-variance investors, a negative

ESG premium arises if the ESG mandate is binding for asset managers. A result that is borne out by the data. Finally, we examine the impact of ESG-controversy events on the stock prices of companies in the S&P100 index, incorporating a Twitter-based sentiment index to quantify social media reputation. Our findings show that ESG controversies negatively affect stock returns, with the impact being inversely related to a company's social media reputation. Companies with stronger reputations experience a shorter, less significant impact, while those with lower reputations face more persistent negative effects, lasting up to four days. Importantly, we find that the market is self-resilient: controversies do not cause spillover effects across the broader market. Instead, affected companies become isolated within the financial network, with their risk profiles decoupling from neighboring firms. This containment prevents systemic risks, highlighting the market's ability to absorb and localize the shocks from ESG controversies. Our results hold even when dividends are included, reinforcing the short-lived nature of these effects for most companies.

# ADVANCED MULTIPHYSICS COMPUTATIONAL MODELS FOR THE VASCULAR MICROENVIRONMENT

**Piermario Vitullo** – Supervisor: Paolo Zunino

Co-Supervisors: Maria Laura Costantino, Andreas Linninger, Luca Possenti, Nicola Rares Franco e Alessandro Coclite

The circulatory system is the set of organs and vessels responsible for the flow of blood through tissues. Microcirculation, which plays a crucial role in both physiological and pathological processes of tissues, represents a key focus of such studies, as it governs essential functions, including the transport and exchange of thermal energy, respiratory gases, nutrients, waste products, water, and hormones. The vascular microenvironment (VME) is a complex system influenced by mechanical, hemodynamic, and regulatory factors. The ability to accurately model VME is critical for advancing both fundamental research and clinical applications, such as cancer therapy, cardiovascular disease, and personalized medical treatments. This work is particularly focused on tumor modeling. The models we develop are crucial for studying the pathophysiology of the tumor microenvironment. A comprehensive understanding of microcirculation requires the integration of various measurement techniques. Mathematical models provide a framework for interpreting

experimental data and integrating in-vivo and ex-vivo information. Given the complexity of microcirculation, advanced computational models have become an essential tool for studying biological phenomena related to the microvasculature. Traditional numerical methods are inadequate for this task because of the inherent complexities of the VME, which involve interactions among physical processes across various spatial scales. As a result, the computational burden is excessively high, restricting the feasibility of a forward approach. This thesis aims to address these challenges by developing advanced computational models for studying microcirculation, leveraging on a high-fidelity mixed-dimensional modeling framework to describe blood flow and oxygen transport, coupling complex vascular networks with the surrounding biological tissue. In the first part of the work, the geometrical modeling of a vascular network is addressed. We propose two methods for the synthesis of vascular networks: the first one relies on Voronoi-based diagrams to control

morphometrical and topological properties, while the second approach uses deep learning techniques to create complex and anatomically consistent vascular geometries efficiently. These models are then applied to radiotherapy (RT) to explore how hypoxia affects tumor resistance to radiation. Computational studies show that regions with irregular vascularization exhibit hypoxia and greater radioresistance (Fig.1). Consequently, a sensitivity analysis identifies key factors that influence oxygenation, with a focus on vascular topology. In the second part of the work, we introduce advanced nonlinear reduced-order modeling (ROM) techniques and deep learning approaches to

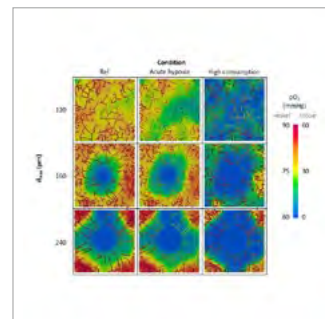


Fig. 1 - Oxygen partial pressure in the tissue and microvascular domains. Regions with irregular vascularization exhibit hypoxia.

achieve a relevant speed-up and a negligible loss in accuracy with respect to the high-fidelity full order model. Based on the standard proper orthogonal decomposition (POD) approach and leveraging Mesh-Informed Neural Networks (MINNs), the ROM combines together a neural network approximating the POD coefficients and a closure model acting as fine-scale corrector for the local structures not captured by the former (Fig.2). This approach is validated by means of an a-priori error analysis. The reduced-order framework allows for efficient computational studies that

require a relevant number of numerical simulations, such as uncertainty quantification and sensitivity analysis, which are essential for assessing the robustness of the physics-based model and a comprehensive understanding of the biological processes studied. In this scenario, we introduce a multifidelity framework to optimally manage the high-fidelity and low-fidelity solvers depending on the available computational resources, balancing the trade-off between computational cost and accuracy. A deep learning-enhanced multifidelity Monte

Carlo (DL-MFMC) method is proposed to accelerate the statistics of quantities of interest, particularly in the context of oxygen transport and RT outcome (Fig.3). The integration of deep learning into these frameworks significantly improves computational performance, enabling large-scale simulations while maintaining accuracy. The final goal is to exploit the developed methodologies and the models to construct a unique framework for real-time robust predictions that can be easily adapted to support clinical decision-making, in particular, referring to personalized clinical treatment of cancer patients. Preliminary applications of these computational models in lab-on-chip systems are explored, analyzing vascular permeability before and after RT. The combination of the lab-on-chip for microcirculation and the advanced computational tools allows the in-silico replica of the in-vitro experiments based on chip, and the merging of experimental data with mechanistic physiologic knowledge in real-time to produce personalized, quantitative predictions that can lead to improved treatments.

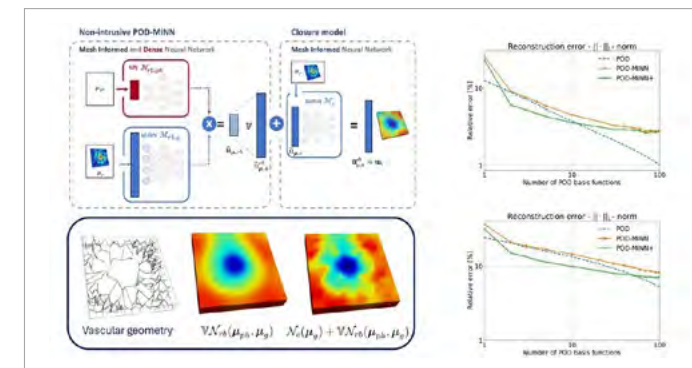


Fig. 2 - Sketch of the POD-MINN+ method.

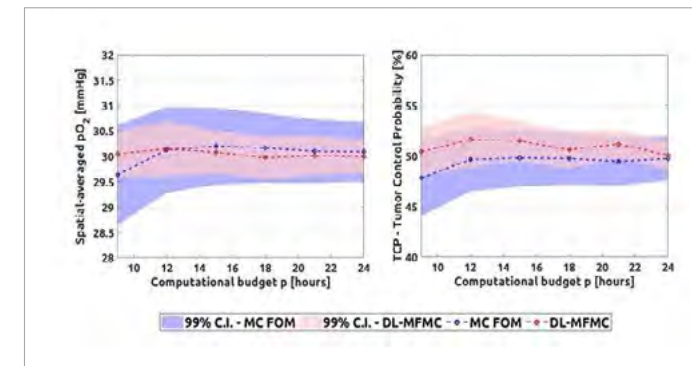


Fig. 3 - Confidence intervals estimates, comparing the DL-MFMC estimator with the standard Monte-Carlo FOM-based.

# NUMERICAL METHODS FOR EPIDEMIC FORECAST AND CONTROL

**Giovanni Ziarelli** – Supervisor: Marco Verani

**Co-Supervisor: Nicola Parolini**

Despite significant progress in virology and epidemiology in preventing and predicting the spread of infectious diseases, many outbreaks—from the common flu to HIV, COVID-19, and monkeypox—have continued to threaten global health over the past few decades. These diseases not only pose a direct health risk but also have far-reaching social and economic repercussions. Consequently, there has been a growing demand for more accurate tools and techniques to forecast disease spread and assess the effectiveness of pharmaceutical and non-pharmaceutical interventions. Mathematical modeling has played a crucial role in addressing these challenges, offering valuable insights into the biological and epidemiological mechanisms of infectious diseases and supporting policymakers in evaluating containment strategies. Advancing in this direction is essential to shedding light on key aspects of disease transmission that remain partially unknown. This thesis contributes to these efforts by developing innovative mathematical models and numerical methods to address unresolved issues, enabling faster and more effective

responses to emerging diseases. Specifically, we focus on three key challenges encountered during epidemic events and propose novel approaches for each:

- Predictions and scenario analyses;
- Controllability of epidemic waves;
- Exploration of transmission mechanisms.

**Predictions and Scenario Analyses**

Beyond quantitative forecasting, scenario analyses provide fundamental qualitative insights that policymakers use to enhance public awareness and evaluate intervention strategies. In this context, surrogate models—especially those leveraging operator learning techniques—play a pivotal role. Our work

focuses on a novel approach within this framework: Kernel Operator Learning (KOL), designed for population dynamics during epidemic outbreaks. This method associates an input strategy (e.g., a measure of NPIs) with the transmission rate. We demonstrate that KOL approaches outperform standard operator learning techniques in terms of computational efficiency for training and testing. Using synthetic but semi-realistic data, we show that these methods enable fast and robust forecasting and scenario analysis. Moreover, they prove competitive in optimizing intervention strategies based on specific performance measures, as confirmed through an extensive campaign of numerical simulations.

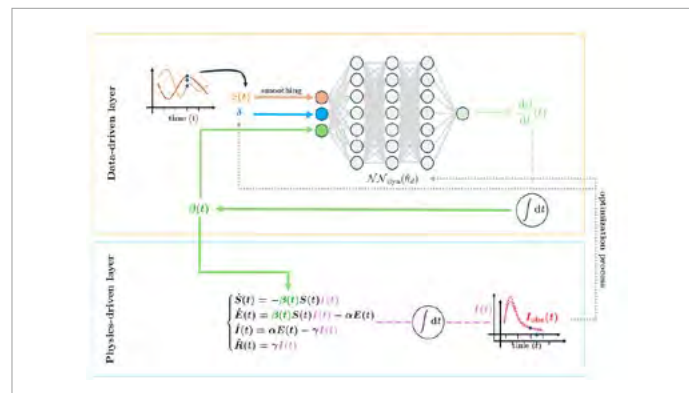


Fig. 1 - Schematic representation of the method.

## Controllability of Epidemic Waves

The controllability of infectious diseases encompasses all medical and non-pharmaceutical interventions aimed at containing or eradicating epidemics. Mathematically, effectiveness has typically been measured using reproduction numbers and growth rates within epidemic models.

This thesis introduces an optimal control framework in which the epidemic model represents state dynamics, while administered vaccine doses serve as control variables. The problem is formulated for the first six months of 2021 and solved numerically to determine improved vaccination strategies compared to the actual dose allocations. The goal is to minimize infections, deaths, and hospitalizations. For this purpose, we develop an age-stratified *SIR*-like compartmental model tailored to two-dose COVID-19 vaccination campaigns. Unlike other models, ours incorporates all disease stages, including death and recovery, while avoiding unnecessary compartments that would increase computational complexity without added relevance. Many numerical simulations, calibrated using data from the Italian Civil Protection Department, validate our framework within the Italian context. Our findings suggest that allocating more doses to individuals aged 20 to 59 helps reduce infections and hospitalizations, whereas

prioritizing those over 80 minimizes recorded deaths. Across all considered scenarios, our optimization framework achieves significant improvements in reducing deaths, infections, and hospitalizations compared to baseline vaccination policies.

## Identification of Hidden Parameters through Machine Learning

The majority of parameters involved in standard epidemic models have clear physiological interpretations and can be estimated via statistical inference on clinical trials or cohort studies. However, transmission-related parameters often depend on harder-to-retrieve data, such as contact rates between infectious and susceptible individuals or the intrinsic transmissibility of a disease. Inaccurate extrapolations of these factors can severely impact forecast quality. We focus on the transmission rate and model its dependence on external measurable quantities—referred to as exogenous variables—through a hybrid approach combining a data-driven layer and a physics-based epidemic model (cf. Figure 1). The data-driven layer employs a neural ordinary differential equation (ODE) to learn the transmission dynamics, conditioned on meteorological data and wave-specific latent parameters, inferred via data assimilation. The physics-based layer consists of a standard *SEIR* compartmental model, where the transmission rate serves as

an input. The learning strategy follows an end-to-end approach, with a loss function quantifying the discrepancy between actual infection data and model predictions. Applying this model to real-world data, we use meteorological information and influenza case reports from Italy (2010–2020). Despite the limited number of training series available, the model generalizes well to observed case data. Moreover, the learned transmission law aligns with established findings, confirming expected dependencies on external factors: drier and warmer conditions correlate with reduced transmission rates. In summary, this thesis introduces novel mathematical and computational tools for epidemic modeling, contributing to more effective prediction, control, and understanding of infectious disease dynamics.