Scientific Machine Learning, emerging topics

18–21 June 2024

SISSA, International School for Advanced Studies, Trieste, Italy

BOOK OF ABSTRACT

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Conference description and location

"Scientific Machine Learning, emerging topics" is an international conference focused on the study of mathematical theory and algorithms of machine learning, and applications of machine learning in scientific computing and engineering disciplines. Particular emphasis will be on

- optimization,
- physics-informed learning,
- graph neural networks,
- neural operators,
- transformers,
- neural odes,
- generative models.

Location: SISSA

SISSA, International School for Advanced Studies, main campus, Trieste, Italy
Main Campus, Building A
Room 128-129, first floor
Via Bonomea 265, 34136 Trieste, Italy.

About SISSA

SISSA, the International School for Advanced Studies, was founded in 1978 and is a scientific center of excellence within the national and international academic scene. Located in Italy, in the city of Trieste, it features 90 professors, about 150 post-docs, 330 PhD students and 115 technical administrative staff. Situated on the scenic Karst upland, the School is surrounded by a 25 acre park, and offers a stunning view of the Gulf of Trieste.

The three main research areas of SISSA are Physics, Neuroscience and Mathematics. All the scientific work carried out by SISSA researchers is published regularly in leading international journals with a high impact factor, and frequently in the

most prestigious scientific journals such as Nature and Science. The School has also drawn up over 150 collaboration agreements with the world's leading schools and research institutes.

The quality level of the research is further confirmed by the fact that within the competitive field of European funding schemes SISSA holds the top position among Italian scientific institutes in terms of research grants obtained in relation to the number of researchers and professors. Such leadership should also be seen in terms of SISSA is ability to obtain funding, both from the private and public sectors, such as FIR and PRIN.

As for the National assessment of research quality involving all Universities and scientific institutes, SISSA got top marks in mathematics and neuroscience, and came first among medium-sized departments in the field of physical science.

See also the official SISSA website www.sissa.it for additional information.

How to reach Trieste

- **By Airplane**: Airports info (Venice and Trieste Airports)
  Connections with intercontinental/international flights may be found in Rome (FCO), by ITA airways, or Frankfurt (FRA) by Lufthansa to/from Trieste Airport (TRS), several flights per day, or in Paris (CDG) / Amsterdam (AMS) / Berlin (TXL)/ AbuDhabi (AUH) to/from Venice Airport (VCE). From Venice to Trieste a fast regional train takes almost 2h. If you land in Trieste airport (TRS) a "Transfer-sharing" service is available on demand and it is named Science-Bus. Thanks to this service, from the airport you will directly reach SISSA or your hotel. This service must be booked on-line, no later than two days before, on the following website www.science-bus.com, where you will find the reservation form to be filled in.

- **By Ground Trasportation**: Stations info and connections (trains/buses)
  High speed trains run from Torino, Milano and Venice to Trieste (FrecciaArgento) or from Rome, Florence, Bologna and Venice to Trieste (Freccia). Fast Regional Trains are available from Venice (Mestre). Trieste is also connected daily to several Italian and European cities by an intercity bus service. The service is provided by the flixbus company.

- **By Car**: Local info Highway A4 runs from Torino, Milano and Venice to Trieste and connects highways from Austria and Germany (Tarvisio, Brennero) as well as national highways from south. More info can be found here.

How to reach SISSA from Trieste

A connection to SISSA campus will be guaranteed by shuttle bus with the following from Piazza Oberdan and SISSA campus:

Piazza Oberdan $\Longrightarrow$ SISSA

- June 18: 1:00pm
- June 19: 8:45am
- June 20: 8:45am
- June 21: 8:45am

SISSA $\Longrightarrow$ Piazza Oberdan

- June 18: 6:30pm
- June 19: 7:30pm
- June 20: 6:30pm
- June 21: 1:10pm

Moreover, SISSA campus can be reached by local public transportation via bus line 38 from Piazza Oberdan every 20 minutes (a valid ticket could be purchased at the vending machine outside SISSA or contactless on board for 1,45€).

Hotels in Trieste

SISSA has special discounted rates with the hotels at this link. Please ask for the special fare directly when booking the hotel.

Programme

Timeslot	Tuesday 18th June	Wednesday 19th June	Thursday 20th June	Friday 21st June
9:30-10:30		Klawonn (p. 15)	Schwab (p. 19)	Cairoli (p. 24)
10:30-11:00		Coffee Break	Coffee Break	Coffee Break
11:00-11:30		Meneghetti (p. 15)	Regazzoni (p. 19)	Propp (p. 25)
11:30-12:00		Pagani (p. 16)	D'Inverno (p. 20)	Marcuzzi (p. 25)
12:00-12:30		Chinellato (p. 17)	Imperatore (p. 21)	Mohammadizadehsorouei (p. 26)
12:30-12:45	Registration	Lunch	Lunch	Closing
12:45-14:00	Registration	Lunch	Lunch	
14:00-14:30	Opening	Lunch	Lunch	
14:30-15:30	Laudato (p. 12)	Pezzuto (p. 17)	Siettos (p. 21)	
15:30-16:00	Randone (p. 12)	Pichi (p. 18)	Coscia (p. 23)	
16:00-16:30	Centofanti (p. 13)	Barletta (p. 19)	Brivio (p. 23)	
16:30-17:00	Coffee Break	Coffee Break	Coffee Break	
17:00-17:30	Millevoi (p. 13)	Posters (p. 27)	Industrial Panel	
17:30-18:00	Ortali (p. 14)	Posters	Industrial Panel	
18:30-19:00		Posters		

Oral Presentations

Deciphering Thrombosis: Advancing Multi-Scale Modeling with THRONE

Tuesday, 18th June, 14:30-15:30

Marco Laudato

Affiliation: KTH Royal Institute of Technology

Contribution type: Keynote speaker

Keywords: DeepONet, Thrombosis, Multi-scale, CFD, DPD

Abstract

The THRONE (Thrombosis Operator NEtwork) project pioneers a novel approach to understanding thrombosis through the lens of multi-scale modeling, leveraging the power of Deep Operator Networks (DeepONet). By integrating Dissipative Particle Dynamics (DPD) simulations with advanced machine learning techniques, THRONE aims to predict the complex behavior of blood flow and platelet aggregation leading to thrombus formation. At its core, the project develops a surrogate model capable of accurately simulating the micro-mechanical interactions within blood under various flow conditions, specifically focusing on the critical role of platelets. Utilizing the Couette flow to represent shear stress conditions in blood vessels, THRONE captures the essence of thrombus development in stenotic regions.

SOGA: Second Order Gaussian Approximation of Probabilistic Programs

Tuesday, 18th June, 15:30-16:00

Francesca Randone

Affiliation: University of Trieste

Contribution type: Speaker

Keywords: Generative models, probabilistic programming, Gaussian approximation

Abstract

Probabilistic programming is a rising paradigm, that allows specifying generative models by using ad hoc programming languages augmented with probabilistic primitives and running a number of off-the-shelf inference algorithms on them, including Monte Carlo Markov chain sampling, quantization, symbolic execution, and variational inference. SOGA (Second Order Gaussian Approximation), is a Python-based tool that performs inference using an analytical approximation that leverages the approximating power of Gaussian Mixtures (GMs) and moment-matching. It represents the joint probability distribution of the program variables at each location by means of multivariate Gaussian mixtures (GMs), matching the first two-order moments of the true probability distribution. SOGA supports both continuous and discrete distributions and data-based inference. Moreover, it has been shown to offer better scalability than sampling-based and symbolic methods on some classes

of models. I will present an overview of SOGA, applications to models taken from different fields and possible new research directions.

Operator Learning for Ionic Models in Biomathematics

Tuesday, 18th June, 16:00-16:30

Edoardo Centofanti

Affiliation: Università degli Studi di Pavia

Contribution type: Speaker

Keywords: Operator Learning, DeepONet, Neural Operators

Abstract

Ionic models are among the most extensively studied dynamical systems in biomathematics, as they play a crucial role in modelling electrophysiology at the cellular scale. In particular, they are a crucial component in cardiac modelling since they account for the excitability of the cellular membrane and they are responsible for the action potential. Since they may significantly contribute to the computational complexity of the problem, it is important to develop alternative techniques that minimize their impact on the global solution time. In this talk, we will introduce a strategy for exploiting Operator Learning techniques, such as DeepONet, Fourier Neural Operator (FNO) and Wavelet Neural Operator (WNO), to solve these systems more efficiently. Specifically, we will compare the accuracy of the trained models with the ones solved numerically and discuss the capabilities of these architectures in reconstructing the desired dynamics.

DeepONet-based inverse approximator in matrix-free applications

Tuesday, 18th June, 17:00-17:30

Caterina Millevoi

Affiliation: University of Padova

Contribution type: Speaker

Keywords: DeepONet, inverse approximation, preconditioner

Abstract

Preconditioners are widely used for solving differential equations iteratively and one popular preconditioner that can parallelize the calculation is the inverse approximation. However, for high-dimensional system matrices, computing such preconditioners is not practical. We provide a method for computing approximate inverses by using DeepONet, a supervised tool that can be trained to learn nonlinear operators. In order to approximate the action of the inverse of the system matrix, we build a DeepONet with particular input layers to make it aware of the mesh coming from

the problem discretization. The proposed method is validated on test cases, offering a novel way to approximate the inverse of discrete operators.

Tuesday, 18th June, 17:30-18:00

Turbulence Subgrid Closure for the Lattice Boltzmann Method via Artificial Neural Networks

Giulio Ortali

Affiliation: Eindhoven University of Technology, SISSA International School for Advanced Studies

Contribution type: Speaker

Keywords: Lattice Boltzmann Method, Neural Networks, Physics Informed Machine Learning, Turbulence

Abstract

This work introduces a novel approach to learning Turbulence Subgrid Closure models within the context of Lattice Boltzmann Method using physics-constrained Artificial Neural Networks.

The Lattice Boltzmann Method (LBM) is a class of computational methods, stemming from the kinetic theory of gases, used to simulate the dynamics of fluid flows at the mesoscopic level. The fluid is represented via the dynamics of a set of discrete particle distribution functions (populations). These populations evolve according to the stream and collide algorithm, where at each time step populations hop from lattice-site to lattice-site and then incoming populations collide among one another. We work in the context of 3D Homogeneous Isotropic Turbulence on a cube with periodic boundary conditions, considering a fully resolved setting, generating ground truth Direct Numerical Simulation (DNS) data, and different coarse graining factors.

We learn a novel collisional term, expressed as a correction to the BGK collisional operator, using a physics-constrained Artificial Neural Network trained on DNS data. The model comprises a standard Multi-Layer Perceptron, followed by post-processing layers enforcing mass and momentum conservation, trained on multi-step prediction.

The proposed model shows promising results, closely capturing both energy spectra and higher-order statistics of filtered DNS data compared to traditional techniques such as the Smagorinsky turbulence model. Remarkably, our approach is fully local both in space and time, leading to reduced computational costs, enhanced generalization capabilities and interpretability. Additionally, this formulation can be in principle used to learn any new collisional operator, given the proper ground truth data, and to acquire a deeper understanding in the physics of turbulent flows.

Domain Decomposition Methods and Machine Learning - Two Mutually Beneficial Areas

Wednesday, 19th June, 9:30-10:30

Axel Klawonn

Affiliation: Universitaet zu Koeln

Contribution type: Keynote speaker

Keywords: convolutional neural networks, model parallelism, parallel training, image classification, domain decomposition, scientific machine learning

Abstract

Hybrid algorithms, which combine black-box machine learning methods with experience from traditional numerical methods and domain expertise from diverse application areas, are progressively gaining importance in scientific machine learning and various industrial domains, especially in computational science and engineering.

In this talk, we consider the mutually beneficial combination of machine learning (ML) and domain decomposition methods (DDMs). We give an overview of existing work within this field and classify it into domain decomposition for machine learning and machine learning-enhanced domain decomposition, including: domain decomposition for classical machine learning, domain decomposition to accelerate the training of physics-aware neural networks, machine learning to enhance the convergence properties or computational efficiency of DDMs, and machine learning as a discretization method in a DDM for the solution of PDEs. Highlighting examples will be presented for a number of the aforementioned research areas.

This talk is based on joint work with Martin Lanser and Janine Weber, University of Cologne, Germany.

A Reduced Order Approach for Artificial Neural Networks applied to Object Recognition

Wednesday, 19th June, 11:00-11:30

Laura Meneghetti

Affiliation: SISSA

Contribution type: Speaker

Keywords: object recognition, neural networks, dimensionality reduction, tensor decomposition

Abstract

Computer Vision is a thriving field increasingly exploited in several scientific and engineering contexts in order to solve complex tasks such as the recognition and detection of objects inside pictures. A possible approach to deal with image processing problems is represented by Convolutional Neural Networks (CNNs). Such architectures well perform on complex tasks such as object recognition but may require a high number of layers to extract all the features of the problem at hand,

leading to more parameters to be calibrated during the training phase. This naturally opens several computational issues in the learning procedure, as well as in the memory and space required by the model itself, especially in the case these networks have to operate in vision devices with limited hardware. A possible solution for the aforementioned problem is represented by the development of a dimensionality reduction technique for CNNs by employing Proper Orthogonal Decomposition (POD), a method widely used in the context of Reduced Order Modeling, or Higher Order SVD (HOSVD), to keep into account the intrinsic tensorial structure. The reduced network is then obtained by splitting the original one in two different nets connected by the reduction technique: the first one obtained by retaining a certain number of layers of the original model and a second one that deals with the classification of the features extracted by the previous part. In our works we propose several version of reduced networks to tackle two different problems: image recognition and object detection. For the first case, we provide the numerical results obtained by applying such method to benchmark CNNs, such as VGG-16 and ResNet-110, using CIFAR-10, CIFAR-100 and a custom dataset. For the object detection case, we present a possible generalization of the method proposed for Artificial Neural Networks to object detectors and in particular to SSD-300 or neural networks with a similar architecture. We then provide the results obtained by training our reduced model against the PASCALVOC dataset.

Wednesday, 19th June, 11:30-12:00

Deep learning approaches for meshless surrogate models in variable geometries

Stefano Pagani

Affiliation: MOX-Dipartimento di Matematica, Politecnico di Milano

Contribution type: Speaker

Keywords: Neural Networks, Implicit Neural Representations, Features Encoding, Surrogate Models

Abstract

Efficient numerical models are essential in many engineering applications to explore system response to design modifications in material properties and geometry. Standard modeling and simulation approaches, which involve the generation of computational grids and the numerical discretization of parameterized partial differential equations, are often computationally impractical. Instead, surrogate data-driven models based on neural networks are preferred for their enhanced computational efficiency. However, designing training strategies to achieve optimal generalization capabilities remains an open challenge, especially when dealing with high parametric and geometric variability.

In this talk, we present a technique that combines neural network models to reconstruct both the domain and associated parametric PDE solutions. First, we train a neural network to generate a shape model encoding geometric variability. To

avoid relying on computational meshes, we employ an implicit representation that only necessitates knowledge of point data that belongs to the geometry's surface. Then, we train a second neural network to reconstruct spatiotemporal quantities of interest while incorporating geometry dependence through appropriate feature encodings linked to the first neural network.

This work is in collaboration with F. Regazzoni (Politecnico di Milano), D. Carrara (Università di Trento) and S. Pezzuto (Università di Trento).

Deep unfolding for matrix factorizations

Wednesday, 19th June, 12:00-12:30

Erik Chinellato

Affiliation: Università degli Studi di Padova

Contribution type: Speaker

Keywords: Deep-unfolding, Physics-aware, NMF

Abstract

In the context of machine learning, the deep unfolding technique allows to construct highly interpretable neural networks (NNs) characterized by computationally undemanding inference procedures, effectively striking a balance between model-based methods and deterministic deep networks. In this talk we give a general presentation of the deep unfolding concept, its flexibility and predisposition to bring about physics-aware NNs. We will then provide some exemplar applications involving specifically matrix factorizations, e.g. Nonnegative Matrix Factorization (NMF).

Δ-PINNs: physics-informed neural networks on complex geometries

Wednesday, 19th June, 14:30-15:30

Simone Pezzuto

Affiliation: Università di Trento

Contribution type: Keynote speaker

Keywords: PINN, positional encoding, irregular domains, eigenfunctions

Abstract

In this talk I will present a novel positional encoding mechanism for PINNs based on the eigenfunctions of the Laplace-Beltrami operator. This technique allows to create an input space for the neural network that represents the geometry of a given object. We extensively test and compare the proposed methodology against traditional PINNs in complex shapes, such as a coil, a heat sink and a bunny, with different physics, such as the Eikonal equation and heat transfer. We also study the sensitivity of our method to the number of eigenfunctions used, as well as the

discretization used for the eigenfunctions and the underlying operators. Our results show excellent agreement with the ground truth data in cases where traditional PINNs fail to produce a meaningful solution. We envision this new technique will expand the effectiveness of PINNs to more realistic applications.

Graph-based machine learning approaches for model order reduction

Wednesday, 19th June, 15:30-16:00

Federico Pichi

Affiliation: SISSA

Contribution type: Speaker

Keywords: Graph neural networks, convolutional autoencoders, reduced order models, multi-fidelity

Abstract

The development of efficient reduced order models (ROMs) from a deep learning perspective enables users to overcome the limitations of traditional approaches [1, 2]. One drawback of the approaches based on convolutional autoencoders is the lack of geometrical information when dealing with complex domains defined on unstructured meshes. The present work proposes a framework for nonlinear model order reduction based on Graph Convolutional Autoencoders (GCA) to exploit emergent patterns in different physical problems, including those showing bifurcating behavior, high-dimensional parameter space, slow Kolmogorov-decay, and varying domains [3]. Our methodology extracts the latent space's evolution while introducing geometric priors, possibly alleviating the learning process through up- and down-sampling operations. Among the advantages, we highlight the high-generalizability in the low-data regime, and the great speedup. Moreover, we will present a novel graph feedforward network (GFN), extending the GCA approach to exploit multifidelity data, leveraging graph-adaptive weights, enabling large savings, and providing computable error bounds for the predictions [4].

References:

[1] Lee, K. and Carlberg, K.T. Model reduction of dynamical systems on nonlinear manifolds using deep convolutional autoencoders. Journal of Computational Physics, 404, p. 108973, 2020.

[2] Fresca, S., Dedé, L. and Manzoni, A. A Comprehensive Deep Learning-Based Approach to Reduced Order Modeling of Nonlinear Time-Dependent Parametrized PDEs. Journal of Scientific Computing, 87(2), p. 61, 2021.

[3] Pichi, F., Moya, B. and Hesthaven, J. S. A graph convolutional autoencoder approach to model order reduction for parametrized PDEs. Journal of Computational Physics, 501, p. 112762, 2024.

[4] Morrison, O., Pichi, F., and Hesthaven, J. S. Graph Feedforward Network: a nonlinear reduction strategy for multifidelity applications. arXiv:2406.03569, 2024.

Learning stability on graphs

Wednesday, 19th June, 16:00-16:30

Antonioreneè Barletta

Affiliation: Spici srl

Contribution type: Speaker

Keywords: Graphs, learning process, neural networks

Abstract

In artificial intelligence applications, the model training phase is critical and computationally demanding. In the graph neural networks (GNNs) research field, it is interesting to investigate how varying the graph topological and spectral structure impacts the learning process and overall GNN performance. In this work, we aim to theoretically investigate how the topology and spectrum of a graph change when nodes and edges are added or removed. Based on this study, a numerical procedure is applied to generate an optimized version of the initial graph. Numerical results highlight stability issues in the learning process on graphs.

Rate estimates of ONets

Thursday, 20th June, 9:30-10:30

Christoph Schwab

Affiliation: SAM ETH

Contribution type: Keynote speaker

Keywords: deep Operator Networks, singularities, multiscales

Abstract

We review new results on emulation rate bounds for ONets for PDEs with particular attention to a) singular perturbations, b) singularities, c) high dimensionality.

Latent Dynamics Networks (LDNets): learning the intrinsic dynamics of spatio-temporal processes

Thursday, 20th June, 11:00-11:30

Francesco Regazzoni

Affiliation: MOX, Dipartimento di Matematica, Politecnico di Milano

Contribution type: Speaker

Keywords: Space-time operator learning, Latent dynamics, Surrogate modeling, Implicit neural representation

Abstract

Predicting the evolution of systems with spatio-temporal dynamics in response to external stimuli is essential for scientific progress. Traditional equations-based approaches leverage first principles through the numerical approximation of differential equations, thus demanding extensive computational resources. In contrast, data-driven approaches leverage deep learning algorithms to describe system evolution in low-dimensional spaces. We introduce an architecture, termed Latent Dynamics Network, capable of uncovering low-dimensional intrinsic dynamics in potentially non-Markovian systems. Latent Dynamics Networks automatically discover a low-dimensional manifold while learning the system dynamics, eliminating the need for training an auto-encoder and avoiding operations in the high-dimensional space. They predict the evolution, even in time-extrapolation scenarios, of space-dependent fields without relying on predetermined grids, thus enabling weight-sharing across query-points. Lightweight and easy-to-train, Latent Dynamics Networks demonstrate superior accuracy (normalized error 5 times smaller) in highly-nonlinear problems with significantly fewer trainable parameters (more than 10 times fewer) compared to state-of-the-art methods.

Thursday, 20th June, 11:30-12:00

Mesh-informed reduced order models for aneurysm risk prediction

Giuseppe Alessio D'Inverno

Affiliation: SISSA

Contribution type: Speaker

Keywords: Aneurysm, WSS, ROMs, Graph Neural Networks

Abstract

The complexity of the cardiovascular system needs to be accurately reproduced in order to promptly acknowledge health conditions; to this aim, advanced multifidelity and multiphysics numerical models are crucial. On one side, Full Order Models (FOMs) deliver accurate hemodynamic assessments, but their high computational demands hinder their real-time clinical application. In contrast, ROMs provide more efficient yet accurate solutions, essential for personalized healthcare and timely clinical decision-making. In this work, we explore the application of computational fluid dynamics (CFD) in cardiovascular medicine by integrating FOMs with ROMs for predicting the risk of aortic aneurysm growth and rupture. Wall Shear Stress (WSS) and the Oscillatory Shear Index (OSI), sampled at different growth stages of the abdominal aortic aneurysm, are predicted by means of Graph Neural Networks (GNNs). GNNs exploit the natural graph structure of the mesh obtained by the Finite Element (FE) discretization, taking into account the spatial local information, regardless of the dimension of the input graph. Our experimental validation framework yields promising results, confirming our method as a valid alternative that overcomes the curse of dimensionality.

Parameterization learning for scattered data adaptive spline fitting

Thursday, 20th June, 12:00-12:30

Sofia Imperatore

Affiliation: University of Florence

Contribution type: Speaker

Keywords: Geometric deep learning, Fitting, Parameterization, Adaptive splines

Abstract

Geometric model reconstruction from scattered or unorganized 3D point clouds is a ubiquitous problem in several applications. Particularly, the input data must be suitably parametrized to be approximated using spline geometric models. In this talk, we present novel geometric deep-learning techniques for parameterizing a scattered point cloud in R^3 on a planar domain based on graph convolutional neural networks. Specifically, we introduce two data-driven parameterization models. The first one predicts the parametric values of the scattered input data from the proximity information of its 3D points and its dual/line graph. The second model is characterized by a novel boundary-informed message-passing input layer that avoids line-graph computation. Finally, we show the effectiveness of these parameterization learning models for adaptive spline fitting with (truncated) hierarchical B-spline constructions.

Solving the inverse problem in complex systems via machine learning: challenges and perspectives

Thursday, 20th June, 14:30-15:30

Constantinos Siettos

Affiliation: Dipartimento di Matematica e Applicazioni "Renato Caccioppoli", Università degli Studi di Napoli Federico II

Contribution type: Keynote speaker

Keywords: Machine Learning, Reduced Order Models, Complex Systems, Tipping Points

Abstract

In recent years, significant advancements in machine learning (ML) have broadened our ability to solve both the forward and, importantly, the inverse problem for dynamical systems with a particular interest in multiscale/complex systems. The solution of the inverse problem for complex systems, all in all, the "discovery" of reduced order models (ROMs) for the emergent dynamics, leverages the ability of novel ML algorithms including physics-informed neural networks (PINNs) and DeepONet, to learn the evolution and solution operators, their parameters and closures among scales, as well as the design of controllers. However, even state-of-the-art ML methodologies, are not without limitations. Their training often involves iterating over a high-dimensional space of parameters, and hyperparameters that can

significantly impact convergence behavior and numerical approximation accuracy. The "curse of dimensionality" grows more due to the complexity of the underlying (unknown) nonlinear operators of the emergent dynamics across scales. Thus, a challenge in contemporary scientific machine learning is to develop novel algorithms that can both discover the hidden macroscopic physical laws, thus bridging scales, and achieve a desired learning accuracy at a low computational cost. Toward to this aim, I will present, a machine learning framework that relaxes the "curse of dimensionality" and uncertainty that characterizes the learning phase of deep-learning schemes, by (a) discovering sets of collective variables/ embeddings for the description of the emergent dynamics on latent spaces, and based on them (b) construct ROMs on the latent-spaces, in order to parsimoniously perform useful numerical tasks, such as the construction of bifurcation diagrams and the identification and uncertainty quantification of tipping points, the control of the emergent dynamics-and—hopefully—obtain additional physical insight. The framework (see e.g. in [1-7]), bridges nonlinear manifold learning, random embeddings, physics-informed neural networks/ Gaussian processes, and the Equation-Free multiscale numerical analysis framework. The illustrative case studies will be (i) an event-driven stochastic agent-based model (ABM) describing the interactions, under mimesis of traders in a simple financial market, (ii) a stochastic ABM of a host-host interaction epidemic evolving on complex networks, (iii) the design of feedback linearization and the design of observers, (iv) the approximation of nonlinear operators of PDEs. Finally, I will discuss some open problems, challenges and perspectives. Some references:

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PINA: a PyTorch Framework for Solving Differential Equations with Deep Learning

Thursday, 20th June, 15:30-16:00

Dario Coscia

Affiliation: SISSA

Contribution type: Speaker

Keywords: Physics Informed Neural Networks, Neural Operators, Reduced Order Models, Machine Learning, Software

Abstract

The last years have seen a growing interest within the scientific computing community to exploit machine learning to address the limitations of conventional methods for solving differential equations. Physics-informed neural network (PINN) and Neural Operator (NO) approaches have emerged as central players due to their promising and innovative approaches to computing differential equations' solutions. In this contribution, we will present a versatile software designed for tackling differential equation learning using PINN and NO methodologies. The package is called PINA, and it is an open-source Python library built upon the robust foundations of PyTorch and PyTorchLightning. It empowers end-users to formulate their problem and craft their models to compute the solution effortlessly. The modular structure of PINA permits it to adapt PINN and NO schemas for user specifics, thus offering the freedom to select the most suitable learning techniques for their particular problem domain. Furthermore, by leveraging the capabilities of the PyTorchLightning package, PINA makes possible the usage of state-of-the-art features for machine learning in the PINN and NO context and adapts to various hardware setups, including GPUs and TPUs. This adaptability makes PINA an ideal candidate for the transition of these methodologies into production and industrial pipelines, where computational efficiency and scalability are of fundamental importance. The contribution will summarize the basic concepts of both methodologies, presenting the package structure to conclude with the solutions of benchmark problems using PINA.

Pre-trained physics-informed deep learning-based reduced order models for nonlinear parametrized PDEs in small data regimes.

Thursday, 20th June, 16:00-16:30

Simone Brivio

Affiliation: Politecnico di Milano

Contribution type: Speaker

Keywords: parametrized PDEs, reduced order modeling, deep learning, pre-training, physics-informed machine learning, small data

Abstract

Deep learning-based reduced order models (DL-ROMs) provide a novel, comprehensive paradigm that supplies fast, efficient and accurate surrogates for simulating nonlinear parametrized PDEs. Recent theoretical and numerical studies argue that the accuracy of such DL-ROMs relies on the design of the involved neural networks, as well as on the amount of labeled data available at the training stage. However, as the PDE complexity increases, so does the required computational burden pertaining to the generation of synthetic data through high-fidelity solvers. For this reason, we are usually able to collect only a handful of labeled data, thus not covering properly the entire parametric space. Physics-informed paradigms have recently emerged in the Scientific Machine Learning literature as they provide a framework to learn parametrized PDEs in an unsupervised manner, namely by leveraging on the underlying physical equations without needing input-output pairs. However, training physics-informed deep learning architectures might be a demanding task that requires substantial computational resources and implies several pitfalls. Within the present talk, we discuss how to integrate the few available labeled data and the underlying physical model to obtain reliable DL-ROMs for simulating nonlinear PDEs in a small data context. Indeed, on one hand we employ a physics-informed loss formulation to compensate for data scarcity, thus feeding the neural network with information about the underlying physics in the regions of the parameter space that are not adequately covered by labeled training data. On the other hand, we aim at employing the available data to accelerate the physics-informed training and to mitigate its peculiar optimization failure modes. Specifically, by intertwining the contributions of data and physics, we devise a novel training paradigm that consists of an efficient pre-training strategy, thus enabling the optimizer to quickly approach the minimum in the loss landscape, and a fine-tuning phase that further enhances the simulation accuracy. Ultimately, we showcase the potential of our approach through suitable numerical experiments involving parametrized PDEs stemming from computational fluid dynamics and mathematical biology.

Towards Reliable and Interpretable Probabilistic Surrogate Models

Friday, 21st June, 9:30-10:30

Francesca Cairoli

Affiliation: Università di Trieste

Contribution type: Keynote speaker

Keywords: Physics-informed learning; Generative Models; Graph Neural Networks

Abstract

Generative models are a powerful tool in deep learning, enabling the inference of surrogate models for complex stochastic systems. Their probabilistic nature facilitates the quantification of predictive uncertainty. However, these models often function as black boxes, lacking interpretability and presenting challenges in terms of reliability.

To enhance reliability, we are developing a framework for certified generation. This framework leverages robust formal verification techniques to conduct perturbation analysis on the computational graph of our surrogate model, ensuring guaranteed output ranges. Conformal quantile inference can also provide similar guarantees. In pursuit of interpretability, we propose a data-driven generative auto-encoding model. This model automatically derives an explicit representation of a Chemical Reaction Network and its stochastic dynamics directly from the data. Black-box components are employed solely to infer the parameters of a fully interpretable surrogate model, thereby enhancing both the transparency and comprehensibility of the generated models. This approach can help formulate hypotheses about the complex mechanisms that may have generated the observed data.

Discovery of Dirichlet-to-Neumann Maps on Graphs via Gaussian Processes

Friday, 21st June, 11:00-11:30

Adrienne Propp

Affiliation: Stanford University

Contribution type: Speaker

Keywords: graphs, Gaussian processes, Dirichlet-to-Neumann maps, surrogate models

Abstract

We present a novel method for learning Dirichlet-to-Neumann maps on graphs using Gaussian processes, focusing on cases where data obeys some conservation constraint from a PDE. We aim to construct a data-driven surrogate model and uncertainty estimates for an entire graph, even when data is only available for a limited subset of nodes and edges. Our approach combines Gaussian processes and discrete exterior calculus to infer a relationship between node and edge values. By optimizing over the reproducing kernel Hilbert space (RKHS) norm and applying a maximum likelihood estimation (MLE) penalty on kernel complexity, we ensure that our surrogate models adhere to relevant conservation laws without excessive complexity. We demonstrate the effectiveness of our method on various datasets, highlighting its potential for scientific applications with limited data.

Unfolding the Kalman Filter iterations in a machine learning framework

Friday, 21st June, 11:30-12:00

Fabio Marcuzzi

Affiliation: Università degli Studi di Padova

Contribution type: Speaker

Keywords: Kalman Filter, scientific machine learning, deep unfolding, deep learning

Abstract

The Kalman Filter is a traditional approach to discrepancy modeling in a state-space representation where the dominant assumption is that the mismatch between model and measurements is given by normally-distributed random variables. A recent research trend is focused on a scientific machine learning reformulation of the Kalman Filter to overcome his known limits. In this talk we analyze this trend, mainly focusing on a new method obtained by unfolding and untying the conventional iterative KF, combined with back-propagation learning, that we call the Deep Kalman Filter.

Friday, 21st June, 12:00-12:30

A comparative review of regression techniques for predicting the physical characteristics of ship engines

Fatemeh Mohammadizadehsorouei

Affiliation: University of Trieste and SISSA

Contribution type: Speaker

Keywords: Neural Network, Deep learning, Regression

Abstract

Recently, the use of sensors has become widespread in the maritime industry, with ship engines being the main sources for gathering data. The widespread adoption of sensor technologies has resulted in the acquisition and retention of significant amounts of engine performance data. As a result, there is an urgent need for predictive models that are skilled at utilizing this abundance of data to provide significant insights. The rise of terminology like "Industry 4.0" highlights the importance of this fundamental change, propelled by the advancement of digitalization and the introduction of revolutionary technologies like Big Data, Machine Learning, Artificial Intelligence (AI), and the Internet of Things (IoT). The main goal of this marine revolution is to increase the amount of automation and develop self-monitoring systems in ship engines. This will enable the creation of intelligent machines that can analyze and diagnose problems on their own, reducing the need for human involvement. This research was carried out in collaboration with Wärtsilä, a ship engine manufacturer, that employs data acquired from many laboratories for ship engine sensors. The data obtained from sensors corresponds to many physical attributes, like pressure, temperature, speed, and so on. This study uses a combination of regression methods, deep learning, and neural networks to forecast the outputs of the engines. We conducted a comparative analysis of several methodologies using the data at our disposal. Linear regression yields outcomes with lower computational time, while parallel multi-layer regression leads tp superior results but requires more computational time. The multi-layer perceptron demonstrates a balance between computational time and relative errors, ultimately making it the preferred choice.

Poster Presentations

Neural oscillators for generalization of physics-informed machine learning

Wednesday, 19th June, 17:30-19:00

Taniya Kapoor

Affiliation: TU Delft

Contribution type: Poster

Keywords: PINN, PIML, Neural ODEs, PDEs, Generalization, Extrapolation

Abstract

A primary challenge of physics-informed machine learning (PIML) is its generalization beyond the training domain, especially when dealing with complex physical problems represented by partial differential equations (PDEs). This work aims to enhance the generalization capabilities of PIML, facilitating practical, real-world applications where accurate predictions in unexplored regions are crucial. We leverage the inherent causality and temporal sequential characteristics of PDE solutions to fuse PIML models with recurrent neural architectures based on systems of ordinary differential equations, referred to as neural oscillators. Through effectively capturing long-time dependencies and mitigating the exploding and vanishing gradient problem, neural oscillators foster improved generalization in PIML tasks. Extensive experimentation involving time-dependent nonlinear PDEs and biharmonic beam equations demonstrates the efficacy of the proposed approach. Incorporating neural oscillators outperforms existing state-of-the-art methods on benchmark problems across various metrics. Consequently, the proposed method improves the generalization capabilities of PIML, providing accurate solutions for extrapolation and prediction beyond the training data.

Data-Driven Variational Reduced Models Using Learned Radial Basis Functions

Wednesday, 19th June, 17:30-19:00

Jonas Actor

Affiliation: Sandia National Laboratories

Contribution type: Poster

Keywords: Drift-diffusion, Whitney forms, scientific machine learning, microelectronics, structure preservation

Abstract

Data-driven physics models, particularly for problems set in high dimensions, often suffer from the requirement to place collocation points in advance: collocation limits the approximation and optimization errors of the underlying model and necessitates a good placement of the initial basis used for the reduced-order model. Instead, we pose a data-driven ROM via a Gaussian radial basis function approximation scheme, where the shape parameters of the Gaussians are informed by data. Our approach

rests fundamentally on the observation that products of Gaussian radial basis functions (RBFs) and their gradients are integrable as polynomial moments of a product distribution with a closed-form expression, allowing us to assemble mass and stiffness matrices in a Gaussian basis without any quadrature error. This straightforward observation enables a meshfree PDE discretization requiring no numerical quadrature, making it suitable for high-dimensional problems where partitioning space is infeasible. A variational problem posed in this Gaussian basis exhibits convergence as the number of Gaussian RBFs is increased. Due to the infinite support of Gaussians, boundary conditions are enforced by penalty, borrowing from Nitsche's Method to mitigate coercivity error and to maintain the exhibited convergence rate. We demonstrate the method on a handful of PDE data recovery problems on a range of geometries, showing the convergence and flexibility of our approach.

Constrained Generative Models for shape parametrisation

Wednesday, 19th June, 17:30-19:00

Guglielmo Padula

Affiliation: SISSA

Contribution type: Poster

Keywords: Shape parametrization, reduction in parameter space, constrained geometries, generative models.

Abstract

We study generative models for shape optimization of complex geometries with a large number of parameters; the objective is also to reduce the number of relevant geometrical parameters, for example for modeling naval hulls, and creating new artificial geometries similar to real data, as there are non-generative techniques for creating new real geometries which respect some constraints, for having fixed volume, but using them can be costly. The real geometries are parametrized by a lesser number of parameters, which in turn increases the performance of reduced order models.

Integrating Molecular Dynamics and Machine Learning Algorithms to Predict the Functional Profile of Kinase Ligands

Wednesday, 19th June, 17:30-19:00

Ivan Cucchi

Affiliation: Università degli Studi di Pavia

Contribution type: Poster

Keywords: Machine Learning, Computational Chemistry, Molecular Dynamics, Kinase Ligands

Abstract

The modulation of protein function via designed small molecules is providing new opportunities in chemical biology and medicinal chemistry. While drugs have traditionally been developed to block enzymatic activities through active site occupation, a growing number of strategies now aim to control protein functions in an allosteric fashion, allowing for the tuning of a target's activation or deactivation via the modulation of the populations of conformational ensembles that underlie its function. In the context of discovery of new active leads, it would be very useful to generate hypotheses for the functional impact of new ligands. Since the discovery and design of allosteric modulators (inhibitors/ activators) is still a challenging and often serendipitous target, the development of a rapid and robust approach to predict the functional profile of a new ligand would significantly speed up candidate selection. Herein, we present different Machine Learning (ML) classifiers to distinguish between potential orthosteric and allosteric binders. Our approach integrates information on the chemical fingerprints of the ligands with descriptors that recapitulate ligand effects on protein functional motions. The latter are derived from Molecular Dynamics (MD) simulations of the target protein in complex with orthosteric or allosteric ligands. In this framework, we train and test different ML architectures, which are initially probed on the classification of orthosteric vs. allosteric ligands for Cyclin Dependent Kinases (CDKs). The results demonstrate that different ML methods can successfully partition allosteric vs. orthosteric effectors (although to different degrees). Next, we further test the models with FDA-approved CDK drugs, not included in the original data set, as well as ligands that target other kinases, to test the range of applicability of these models outside of the domain on which they were developed. Overall, the results show that enriching training dataset with chemical-physics based information on protein ligand dynamic cross-talk can significantly expand the reach and applicability of approaches for the prediction and classification of the mode of action of small molecules.

Optimization of PINNs for improved weights initialization in applied heat transfer problems

Wednesday, 19th June, 17:30-19:00

Kateryna Morozovska

Affiliation: KTH Royal Institute of Technology

Contribution type: Poster

Keywords: weights optimization, heat transfer, PINN

Abstract

In the previous application of PINNs for thermal modelling of power components , the initial weights of the PINN model follow Glorot normal distribution, where the variance includes the number of input and output units. It often results in longer training times for the model to find "good" weights and consequently can cause overfitting when the training time is too long. To overcome this issue we propose

an optimization algorithm that makes a preliminary estimate of the neural networks and provides initial weights and biases as an improved starting point for training initialization. We consider the relationship between inputs and outputs of the whole neural network and we define the objective function of the optimization problem that approaches the NN. The activation function considered in our problem is the hyperbolic tangent (tanh), however, as a simplification, we first consider the unit saturation function for the optimization. With this approach we can observe that the objective function is the residual function of NN, which with PINNs also means the inclusion of the collocation points. We show how this optimization model can be applied to problems based on realistic case studies in thermal design of electric components.

Parameter estimation of the Arrhenius equation with low data availability using PINNs. A case of cellulose aging in mineral oil

Wednesday, 19th June, 17:30-19:00

Federica Bragone

Affiliation: KTH Royal Institute of Technology

Contribution type: Poster

Keywords: Arrhenius equation, PINNs, symbolic regression

Abstract

The degree of polymerization is an indicator of the aging in the insulation system of power components. The problem of aging is studied on an example using cellulose degradation data from power transformers. However, the data availability for this type of problems is usually scarce. The main degradation mechanisms in polymers are hydrolysis, pyrolysis and oxidation, which together can help to estimate the degree of polymerization. An ODE formulation for the relation between the degree of polymerization and the Arrhenius equation describes the ageing of the cellulose immersed in mineral oil. PINNs is used to estimate unknown parameters of the ODE that describe the environmental conditions in the insulation system. After estimating these parameters for the given data, we interpolate the unknown parameters for different water content, temperatures and oxygen levels by training neural networks. Finally, we derived a mathematical formula for the estimated parameters using symbolic regression, that can be used for future reference in estimating the rate parameter of the Arrhenius equation.

Wednesday, 19th June, 17:30-19:00

Scientific Machine Learning for Computationa Fluid Dynamics applied to the automotive use case

Andrea Bonfanti

Affiliation: BMW AG

Contribution type: Poster

Keywords: Scientific Machine Learning, Physics-Informed Neural Networks, Computational Fluid Dynamics, Nonlinear Optimization

Abstract

Numerical Simulations are a vital tool for virtual product development in engineering companies. However, the cost of performing such simulations becomes prohibitively large when high safety, comfort and efficiency standards are expected from the final product. Despite the challenges of this use case, Scientific Machine Learning algorithms are rapidly evolving from the well-known Physics Informed Neural Network architecture and becoming more and more prone to applicability to real-world scenarios. In this talk we delve on the applicability of currently state-of-the-art methods of this field to automotive use cases. In particular, we discuss the current limitations of the existing algorithms and propose innovative solution to bypass those. Finally, we highlight the benefits that such methods can carry in the car producing industry and present those with practical examples applied to the case of aerodynamic simulations.

Wednesday, 19th June, 17:30-19:00

Fractional Physics-Informed Neural Network (fPINNs)

Pavan Pranjivan Mehta

Affiliation: SISSA, International School of Advanced Studies

Contribution type: Poster

Keywords: Fractional calculus, Physics-informed neural networks, Tempered fractional calculus, Inverse problems

Abstract

Fractional calculus is a generalization of classical (integer-order) derivatives, where the order can be arbitrary. Paradoxically, these are nonlocal operators, addressing anomalous diffusion processes. Recently, fractional derivatives have found applications in real world phenomena, such as turbulence (Mehta et. el, 2019; Mehta, 2023). In order to solve for fractional differential equations, fractional physics-informed neural networks (fPINNs) were introduced in Pang et el. (2019) for forward problems. This was further extended for inverse problems in Mehta (2023) for learning the fractional order by developing pointwise fPINNs.

It is to be noted that the underlying stochastic process governed by fractional operators has an infinite second moment, which is not the case for real world scenarios.

Thus, a tempered definition was introduced producing finite second moments; also truncated definitions, which not only has finite second moment but also addresses the computational challenges. Thus, in this presentation, I will also present the algorithms developed in Mehta (2023) for application to both these definitions and numerically determine the equivalence between these two operators. As a result, I will introduce and compute the horizon of nonlocal interactions.

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Real-time optimal control of parametrized systems by deep learning-based reduced order models

Wednesday, 19th June, 17:30-19:00

Matteo Tomasetto

Affiliation: Politecnico di Milano

Contribution type: Poster

Keywords: parametrized optimal control problems, PDE-constrained optimization, reduced order modeling, deep learning

Abstract

Many optimal control problems require suitable strategies in order to steer instantaneously the considered dynamics. Moreover, the control action needs to be updated whenever the underlying scenario undergoes variations, as often happens in applications. Full- order models based on, e.g., Finite Element Method, are not suitable for these settings due to the computational burden. In addition, conventional reduced order modeling techniques, such as the Reduced Basis method, are linear, intrusive, and usually not efficient in addressing nonlinear time-dependent dynamics. We thus propose a nonlinear, non-intrusive Deep Learning-based Reduced Order Modeling (DL-ROM) technique to control rapidly parametrized PDEs under different scenarios. After optimal snapshots generation, dimensionality reduction and neural networks training in the offline phase, optimal control strategies can be retrieved online in real-time for all the scenarios of interest. The speedup and the high accuracy of the proposed approach have been assessed on different PDE-constrained optimization problems, ranging from flow control to thermal active cloaking

Wednesday, 19th June, 17:30-19:00

A Non-asymptotic Analysis of PINN-Optimization for the Poisson Equation in the Kernel Regime

Jonas Nießen

Affiliation: RWTH Aachen

Contribution type: Poster

Keywords: pinn, optimization, optimization bound, ntk, kernel regime

Abstract

In our work, we analyze the optimization of a PINN algorithm in the kernel regime. In this algorithm we use an explicit projection of the weights to a ball around the initialization after each gradient step. Our contribution consists in the statement and proof of a high-probability bound of the average of the empirical loss functions over the iterations. This bound is formulated as a worst-case bound (in terms of the data distribution) and thus independent of the data distribution. In contrast to other works in the NTK Regime, we neither make an assumption on the geometry of the data points nor do we need massive overparametrization.

Wednesday, 19th June, 17:30-19:00

Generative Models Certification

Francesco Giacomarra

Affiliation: University of Trieste

Contribution type: Poster

Keywords: Neural network certification, Generative Models, Score- based diffusion model, Generative Adversarial Network

Abstract

Generative models such as generative adversarial networks, variational auto-encoders and score-based diffusion models have risen in popularity due to their powerful capabilities in generating novel realistic data. Despite their widespread use, these models often lack interpretability. To tackle this issue, we propose a certification method that enhances the transparency and reliability of these models.

Our approach involves perturbing the latent inputs of generators and applying established techniques for neural network certification. This strategy allows us to offer probabilistic guarantees on generating outputs that satisfy certain requirements. We validate the effectiveness and practical applicability of our approach through various case studies, demonstrating significant advancements in the interpretability of generative models.

Assessment of State-of-the-art predictive models for fluid flow problems

Sajad Salavatidezfouli

Wednesday, 19th June, 17:30-19:00

Affiliation: SISSA

Contribution type: Poster

Keywords: Fluid Flow, predictive, LSTM, Transformers, Encoder-only, Teacher-forcing

Abstract

In this study, we conduct a comprehensive assessment of state-of-the-art predictive models for 2D fluid flow problems, focusing on Long Short-Term Memory (LSTM) networks and various transformer architectures. Fluid flow prediction presents a challenging task due to its complex and nonlinear nature, demanding advanced machine learning techniques for accurate forecasting. We begin by defining the architecture of predictive neural networks, highlighting their capabilities in capturing temporal dependencies and spatial relationships, respectively. Leveraging these attributes, we systematically evaluate the performance of LSTM-based models and transformer variants in predicting 2D fluid flow phenomena.

High-Fidelity Wind Turbine Wake Prediction through CNN-based Superresolution Techniques

Kabir Bakhshaei

Wednesday, 19th June, 17:30-19:00

Affiliation: SISSA

Contribution type: Poster

Keywords: CNN, VAWT, wake, super-resolution, machine learning

Abstract

In this paper, we present a novel approach to high-fidelity wind turbine wake prediction using convolutional neural networks (CNN)-based super-resolution techniques. Wind turbine wakes, which significantly impact the efficiency and lifespan of downstream turbines, have traditionally been challenging to model accurately due to their complex, dynamic nature. By employing CNNs to enhance low-resolution computational fluid dynamics (CFD) simulations, our method substantially improves the spatial resolution and predictive accuracy of wake profiles. This advancement allows for more precise predictions of wake characteristics, such as velocity deficits and turbulence intensity, over a range of atmospheric conditions.

Wednesday, 19th June, 17:30-19:00

Physics-Informed Neural Networks, for Ionic Models in Computational Electrophysiology

Luca Pellegrini

Affiliation: University of Pavia

Contribution type: Poster

Keywords: Physics-Informed Neural Networks, Computational Neuroscience, stiff ordinary differential equations

Abstract

Physics-Informed Neural Networks (PINNs) are effective in solving various differential equations but face challenges when applied to some dynamical systems in Computational Neuroscience, particularly in modeling the electrical activity of neurons. These complex dynamical systems, which are described by stiff ordinary differential equations (ODEs), have a very rich dynamics involving different equilibrium points, limit cycles, and their intricate interactions, with nonlinearities across multiple timescales. To address these challeges, specialized architectures, tailored training strategies, and incorporation of domain knowledge are being explored.

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Scientific Machine Learning, emerging topics

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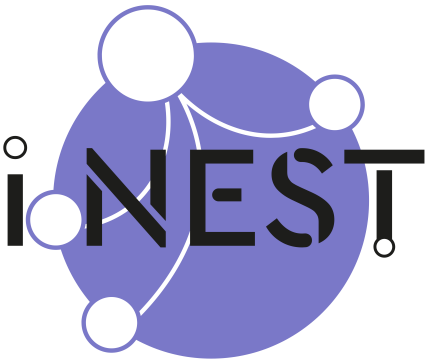

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