



Unione
Matematica
Italiana



Università
degli Studi di
Messina

BOOK OF ABSTRACTS

SS27 - Machine Learning for Numerical Methods in PDEs

2nd Joint Meeting Brazil-Italy in Mathematics

September 10, 2026

Messina, Italy

Organizers:

Alessandro Alla, University of Rome “La Sapienza”
Alvaro Coutinho, Federal University of Rio de Janeiro
Sandra Pieraccini, Polytechnic University of Turin

Augmented predictor–corrector PINN for estimating root zone soil moisture from data at shallower depths

Mariateresa Bruni

Consiglio Nazionale delle ricerche, Istituto di Ricerca sulle Acque, V.le Francesco de Blasio 5,
70132 Bari, Italy

Marco Berardi

Consiglio Nazionale delle ricerche, Istituto di Ricerca sulle Acque, V.le Francesco de Blasio 5,
70132 Bari, Italy

Fabio Difonzo

Libera Università Mediterranea, LUM University Giuseppe Degennaro, S.S. 100 km 18, 70010
Casamassima (BA), Italy

The difficulty of installing soil moisture sensors in the deeper layers of the root zone represents a major limitation for both hydrological modeling and irrigation management. In this study, we propose a predictor–corrector Physics-Informed Neural Network (PINN) framework to estimate soil water content at 60 cm depth using solely measurements collected at 30 cm. The predictor–corrector architecture enables a physically consistent data augmentation strategy, whereby additional informative samples are generated over a depth domain spanning from 0 to 60 cm, allowing the transition from Neumann to Dirichlet boundary conditions and the progressive refinement of the predictions through successive training stages. The results show that the reconstructed soil moisture at 60 cm closely reproduces the observed dynamics, highlighting the capability of the proposed approach to recover soil moisture profiles even in the absence of direct measurements. This methodology therefore provides a practical solution for extending observational datasets in real-world applications, particularly when in situ sensors or satellite products are limited to shallow soil layers.

Neural Preconditioning Strategies for Mixed-Dimensional PDEs: from Static to Dynamic Training

Nunzio Dimola

MOX, Department of Mathematics, Politecnico di Milano.

Alessandro Coclite

Department of Electrical and Information Engineering (DEI). Politecnico di Bari

Paolo Zunino

MOX, Department of Mathematics, Politecnico di Milano.

Mixed-dimensional partial differential equations (PDEs), characterized by couplings between operators defined on domains of different dimensionality, pose significant computational challenges due to their inherent ill-conditioning. Moreover, the computational cost increases substantially when such problems must be solved repeatedly to address multiple instances of the low-dimensional component, which in many practical applications correspond to varying configurations of fracture, fiber, or vascular networks.

In this work, we develop a novel training strategy for neural preconditioners developed in [1] that leverages the geometric structure of Krylov subspace methods. The core contribution is the formulation of a dynamic training algorithm in which the loss functional directly optimizes the angles between Krylov subspaces that govern the convergence behavior of iterative solvers [2].

The proposed approach retains the advantages of unsupervised learning, such as straightforward data generation and independence from ground-truth solutions, while introducing a transparent, solver-integrated performance metric. A differentiable formulation of the Flexible GMRES algorithm enables efficient gradient-based optimization via backpropagation through the solver's iterative process. The resulting dynamic loss captures the alignment between the residual vector and the Krylov subspace at each iteration, providing a geometrically meaningful proxy for the convergence rate.

The performance of this solver-aware training strategy is validated through numerical experiments, which demonstrate a significant acceleration of iterative solver convergence. The method generalizes across different topological configurations of one-dimensional graphs and adapts to variations in problem discretization without requiring retraining.

These results confirm the effectiveness of the proposed training strategy in enabling the neural preconditioner to directly influence Krylov subspace geometry and, consequently, to accelerate the convergence of iterative solvers.

References

- [1] Dimola N., Franco N. R., Zunino P. *An Operator Learning Approach for Preconditioning Mixed-Dimensional PDEs*. Computers and Mathematics with Applications (2025).
- [2] Dimola N., Coclite, A., Zunino P. *Neural Preconditioning via Krylov Subspace Geometry*. Bollettino dell'Unione Matematica Italiana (2025).

Efficient numerical treatment of multidimensional reaction-diffusion PDEs

*Samira Iscaro*¹, *Dajana Conte*

Department of Mathematics, University of Salerno, Fisciano (SA), Italy

Severiano González-Pinto, Domingo Hernández-Abreu

Department of Mathematical Analysis, University of La Laguna, Tenerife, Spain

Giovanni Pagano

Department of Agricultural Sciences, University of Naples Federico II, Portici (NA), Italy

Reaction-diffusion partial differential equations (PDEs) play a central role in the mathematical modeling of complex processes arising in sustainability and energy-related applications, including electrochemical phenomena in batteries, vegetation dynamics, and combustion processes. The reliable numerical simulation of these phenomena requires high-order, stable, and efficient time integration methods, particularly in applications involving repeated large-scale PDE solves within iterative optimization procedures for parameter calibration. Among the available approaches, linearly implicit W methods represent a promising class of integrators [5].

In this talk, we therefore focus on two complimentary goals. First, we investigate strategies to improve the efficiency of the above mentioned W methods. In particular, we combine W-methods of order up to four [1,4,6] with Approximate Matrix Factorization (AMF) and matrix-oriented techniques, exploiting the structure of the matrices generated by the discretization of the diffusion operator by means of finite differences. A detailed comparison of the resulting approaches is carried out in terms of computational cost and accuracy [2].

Secondly, we focus on a more general framework of PDEs with time-dependent boundary conditions. In this setting, W methods may experience the phenomenon of order reduction [4]. To address this issue, we propose new boundary correction techniques aimed at restoring the expected convergence order, with a moderate additional computational effort [3]. The effectiveness of the proposed techniques is assessed on several problems with prescribed Neumann, Robin, or mixed Dirichlet-Neumann boundary conditions in multiple space dimensions.

References

- [1] D. Conte, S. González-Pinto, D. Hernández-Abreu, and G. Pagano. *On approximate matrix factorization and TASE W-methods for the time integration of parabolic partial differential equations*. J. Sci. Comput. 100(2), 34. 2024.
- [2] D. Conte, S. Iscaro, G. Pagano. *On Matrix-Oriented and AMF-W Methods for advection-reaction-diffusion Partial Differential Equations*. In preparation.
- [3] S. González-Pinto, D. Hernández-Abreu, S. Iscaro. *On The Treatment Of Boundary Conditions for AMF-W Methods On Diffusion-Reaction PDEs*. Submitted.
- [4] González-Pinto, S., Hernández-Abreu, D. *Boundary corrections for splitting methods in the time integration of multidimensional parabolic problems*. Appl. Numer. Math., 210: 95-112. 2025.
- [5] Wanner, G., Hairer, E. *Solving ordinary differential equations II*. Vol. 375. New York: Springer Berlin Heidelberg. 1996.
- [6] W. Hundsdorfer, J. G. Verwer. *Numerical solution of time-dependent advection diffusion-reaction equations*. Vol. 33. Springer Science and Business Media., 2003.

¹This talk falls within the activities of PRIN-MUR 2022 project 20229P2HEA "Stochastic numerical modelling for sustainable innovation", CUP: E53D23017940001, granted by the Italian Ministry of University and Research within the framework of the Call relating to the scrolling of the final rankings of the PRIN 2022 call.

E-mail: siscaro@unisa.it.

Hierarchical Clustering and Model Reduction for Optimal Control of ABMs

*Angela Monti*¹, *Fasma Diele*

Istituto per le Applicazioni del Calcolo "M. Picone", CNR, Bari, Italy

Dante Kalise

Department of Mathematics, Imperial College London, UK

Agent-based models (ABMs) describe systems of interacting agents capable of displaying complex collective behaviours such as consensus formation and clustering, with applications in biology and social dynamics [1,2]. However, as the number of agents and the dimension of their states increase, the design of optimal control strategies becomes computationally prohibitive. In this talk, we present a scalable control framework that combines two complementary model reduction strategies: hierarchical clustering, which reduces the number of agents by capturing collective dynamics at the level of cluster centers, and projection-based [3] reduction via Proper Orthogonal Decomposition (POD). These components are integrated within a feedback loop to design optimal control laws on a reduced-order representation of the system. Numerical results on opinion dynamics models [4] show that the proposed approach significantly improves computational efficiency and enables control in regimes where direct methods become infeasible.

References

- [1] F. Cucker, S. Smale, *On the mathematics of emergence*, Japanese Journal of Mathematics 2 (2007), 197–227.
- [2] J. A. Carrillo, D. Kalise, F. Rossi, E. Trélat, *Controlling swarms toward flocks and mills*, SIAM Journal on Control and Optimization 60 (2022), 18631891.
- [3] P. Benner, S. Gugercin, K. Willcox, *A Survey of Projection-Based Model Reduction Methods for Parametric Dynamical Systems*, SIAM Review 57 (2015), 483531.
- [4] R. Hegselmann, U. Krause, *Opinion dynamics and bounded condence: models, analysis and simulation*, Journal of Artificial Societies and Social Simulation 5 (2002).

¹A.M. acknowledges support from a scholarship (*borsa per l'estero*) granted by Istituto Nazionale di Alta Matematica (INdAM) to carry out a research stay at Imperial College London
E-mail: angela.monti@cnr.it.

A Feedback-Control Perspective on Sampling for Langevin and McKean–Vlasov Dynamics

Dante Kalise, Lucas M. Moschen, Grigorios A. Pavliotis
Department of Mathematics, Imperial College London, UK

This talk discusses a feedback-control construction for the N -particle interacting system

$$dX_t^i = -\nabla V(X_t^i) dt - \frac{1}{N} \sum_{j=1}^N \nabla W(X_t^i - X_t^j) dt + \sqrt{2\sigma} dB_t^i, \quad i = 1, \dots, N,$$

where $(B^i)_{i=1}^N$ are independent standard Brownian motions and N is large. The feedback is designed from the mean-field PDE, viewed as the Wasserstein gradient flow of the entropy-regularized free energy

$$\mathcal{F}(\mu) := \mathcal{E}(\mu) + \sigma \int_{\mathbb{T}^d} \mu \log \mu dx.$$

In the case $W \equiv 0$, this is the Fokker–Planck equation associated with the overdamped Langevin dynamics used for sampling from a Gibbs density. The goal is to use feedback as a controlled burn-in mechanism by accelerating convergence of the empirical measure μ_t^N to a selected equilibrium. This is more needed when $\mathcal{F}$ is nonconvex around $\bar{\mu}$, since the small eigenvalues of the Wasserstein Hessian of $\mathcal{F}$ control the convergence rate.

The feedback is built from the eigenfunctions associated with eigenvalues $\lambda_j \leq \delta$ of the Wasserstein Hessian of $\mathcal{F}$ through an algebraic Riccati equation, and it adds to each particle a drift depending only on the empirical averages of those eigenfunctions. For the closed-loop particle system, conditioned consistency on short blocks, positive-time smoothing of the McKean–Vlasov flow, and Gaussian concentration of the particle Itô map give the estimate

$$\sup_{t_{\text{burn}} \leq t \leq e^{c'} N} \mathbb{E} W_2^2(\mu_t^N, \bar{\mu}) \leq C \beta_d(N) + C e^{-(c-c')N}.$$

Here $\beta_d(N)$ is the empirical-measure rate of [3]. Thus the feedback replaces the usual logarithmic-time obstruction by an exponentially long confinement estimate, within the local basin where the PDE stabilization theorem applies.

For sampling, the normalizing constant of the Gibbs density is usually not available. This work shows how the same controller can be assembled from the unnormalized weight e^{-V} , using the fact that the eigenproblem and the selected eigenfunctions are unchanged. Numerical experiments illustrate this implementation. I will also discuss methods for recovering the selected Hessian eigenfunctions from data.

References

- [1] D. Kalise, L. M. Moschen, G. A. Pavliotis, *Feedback Control and Local Convergence of Wasserstein Gradient Flows*, Preprint, 2026.
- [2] A.-S. Sznitman, *Topics in propagation of chaos*, in *École d’Été de Probabilités de Saint-Flour XIX–1989*, Lecture Notes in Math. 1464, Springer, 1991, 165–251.
- [3] N. Fournier, A. Guillin, *On the rate of convergence in Wasserstein distance of the empirical measure*, Probab. Theory Related Fields, 162 (2015), 707–738.

C^0 -Conforming Neural Approximated Virtual Element Method on Polygonal Meshes

Stefano Berrone, Gioana Teora¹

Dipartimento di Scienze Matematiche “G. L. Lagrange”, Politecnico di Torino, Italy

Moreno Pintore

Laboratoire Jacques-Louis Lions, Sorbonne Université, France

We propose two neural-network-based approaches for the construction of C^0 -conforming approximation spaces on general polygonal meshes for the numerical solution of partial differential equations. The proposed techniques are inspired by the Virtual Element Method (VEM) [1], but replace the implicit formulation of local basis functions with explicit neural-network representations to avoid the usage of problem-dependent projection and stabilization operators typically required in VEM. These neural approximations are subsequently employed within a conventional finite element assembly framework.

The original Neural Approximated Virtual Element Method (NAVEM) approximates the VEM basis functions on each element by training neural networks to identify a suitable combination of harmonic functions that mimics the target VEM basis function on the element boundary [2]. However, since the reconstructed basis functions are computed independently on each element, the resulting approximation space is, in general, nonconforming across inter-element boundaries.

To recover C^0 -conformity, we introduce two alternative neural formulations, named B-NAVEM and P-NAVEM, both based on fully connected feed-forward architectures but characterized by different training strategies [3]. In B-NAVEM, the local basis functions are obtained through a Physics-Informed Neural Network (PINN) strategy with strongly enforced Dirichlet boundary conditions. The neural networks are trained to solve the local Laplace problems associated with the VEM basis functions. The resulting basis functions match polynomial VEM traces on the element boundaries and remain approximately harmonic inside the elements, thereby reproducing the main features of the VEM space while ensuring continuity across the mesh. The second approach, P-NAVEM, follows a different philosophy. Rather than reproducing the VEM space itself, it directly learns continuous approximation functions by imposing a polynomial reproducibility condition, which is the essential ingredient for achieving optimal polynomial convergence properties.

Several numerical tests on linear and nonlinear problems confirm that both approaches achieve optimal convergence rates, within the approximation capability of the neural networks, and deliver results comparable to those of the standard VEM, while maintaining the flexibility of polygonal discretizations.

References

- [1] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, A. Russo, *Basic principles of Virtual Element Methods*, Mathematical Models and Methods in Applied Sciences, vol. 23, no. 01, pp. 199–214, 2013. doi: 10.1142/S0218202512500492.
- [2] S. Berrone, M. Pintore, G. Teora, *The lowest-order neural approximated virtual element method on polygonal elements*, Computers & Structures, vol. 314, p. 107753, 2025. doi: 10.1016/j.compstruc.2025.107753.
- [3] S. Berrone, M. Pintore, G. Teora, *Two continuous extensions of the neural approximated virtual element method*, 2026. doi: 10.48550/arXiv.2601.09595.

¹The speaker acknowledges the financial support provided by INdAM-GNCS Project “Metodi numerici politopali stabilization-free e neural-based per problemi accoppiati e non lineari” (CUP: E53C25002010001).

E-mail: gioana.teora@polito.it.