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FRANCE 2030
PROGRAMME DE RECHERCHE
NUMÉRIQUE POUR L'EXASCALE

Exa-MA project
WP2: Model order, Surrogate, Scientific Machine Learning methods

Emmanuel Franck, Macaron project-team
Université de Strasbourg, Centre Inria de l'Université de Lorraine Stéphane Lanteri, Atlantis project-team
Université Clote d'Azur, Inria, CNRS, LJAD, Sophia Antipolis

1. WP2 objectives

WP2 objectives

Two main objectives

- Ultra-fast surrogate models of complex physical problems
- Strategies for leveraging surrogates in multifidelity modeling

Methodological approaches

- Data-driven: reduced basis methods (RBM) and Deep Neural Networks (DNN)
- Model-driven: Physics-Based Neural Networks (PBNN)

WP2 objectives

T2.1 – Surrogate models based on PINNs

T2.2 – PDE operator learning with Neural Operators

T2.3 – Data-driven model order reduction

T2.4 – Non-intrusive reduced basis methods for parametric problems

T2.5 – Multifidelity modeling

T2.6 – Real-time models with super resolution methods

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2. WP2 highlights

WP2 highlights

T2.1 – Surrogate models based on PINNs
Multilevel distributed PINNs for frequency-domain acoustic problems

PhD thesis of Daria Hrebenshchykova (Atlantis@Inria and Macaron@Inria teams)

Key points

- Helmholtz equation in 2D with PML (Perfectly Matched Layers) domain truncation
- FBPINNs (Finite Basis PINNs): Schwarz type domain decomposition
- MFBPINNs: multilevel version
- Implemented in Scimba
- Energy Nature Gradient (ENG) optimization method

Dissemination

- DD29 presentation, Milano, June 2025 (paper accepted in proceedings)

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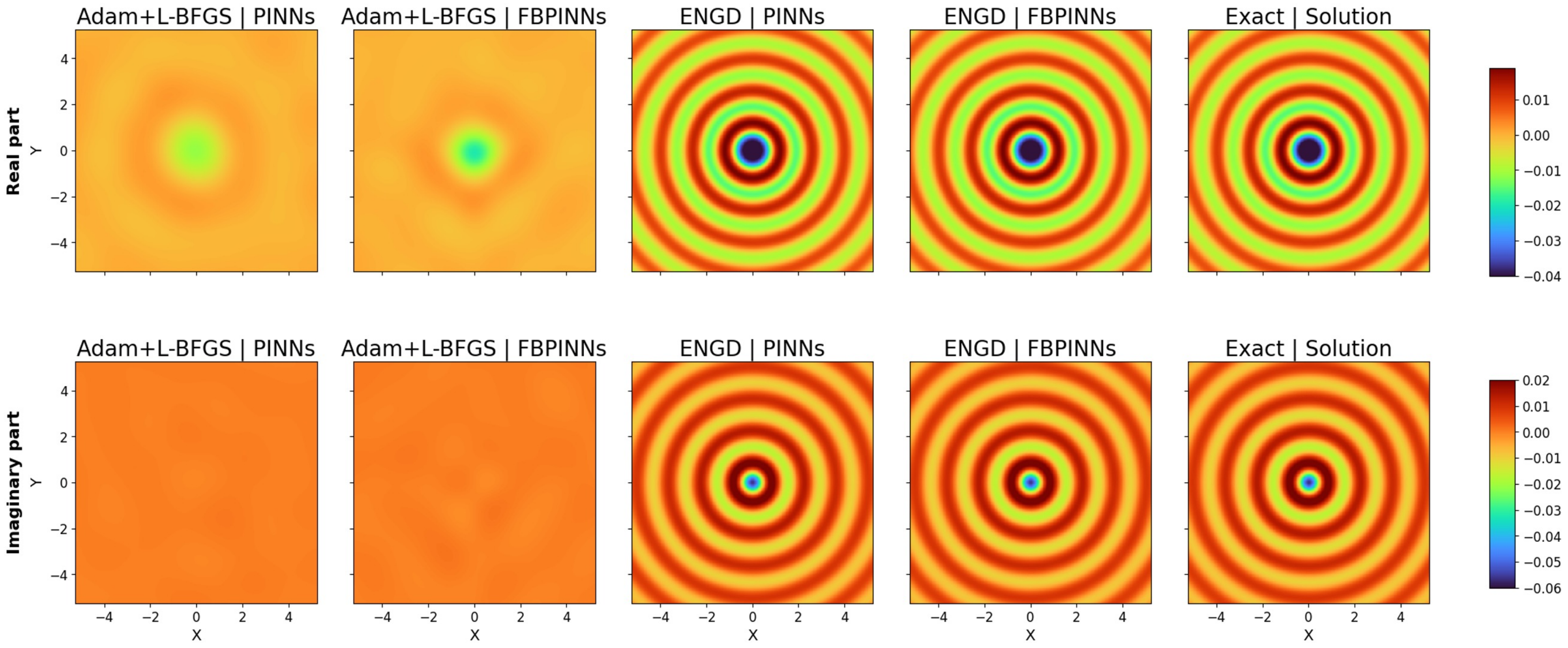
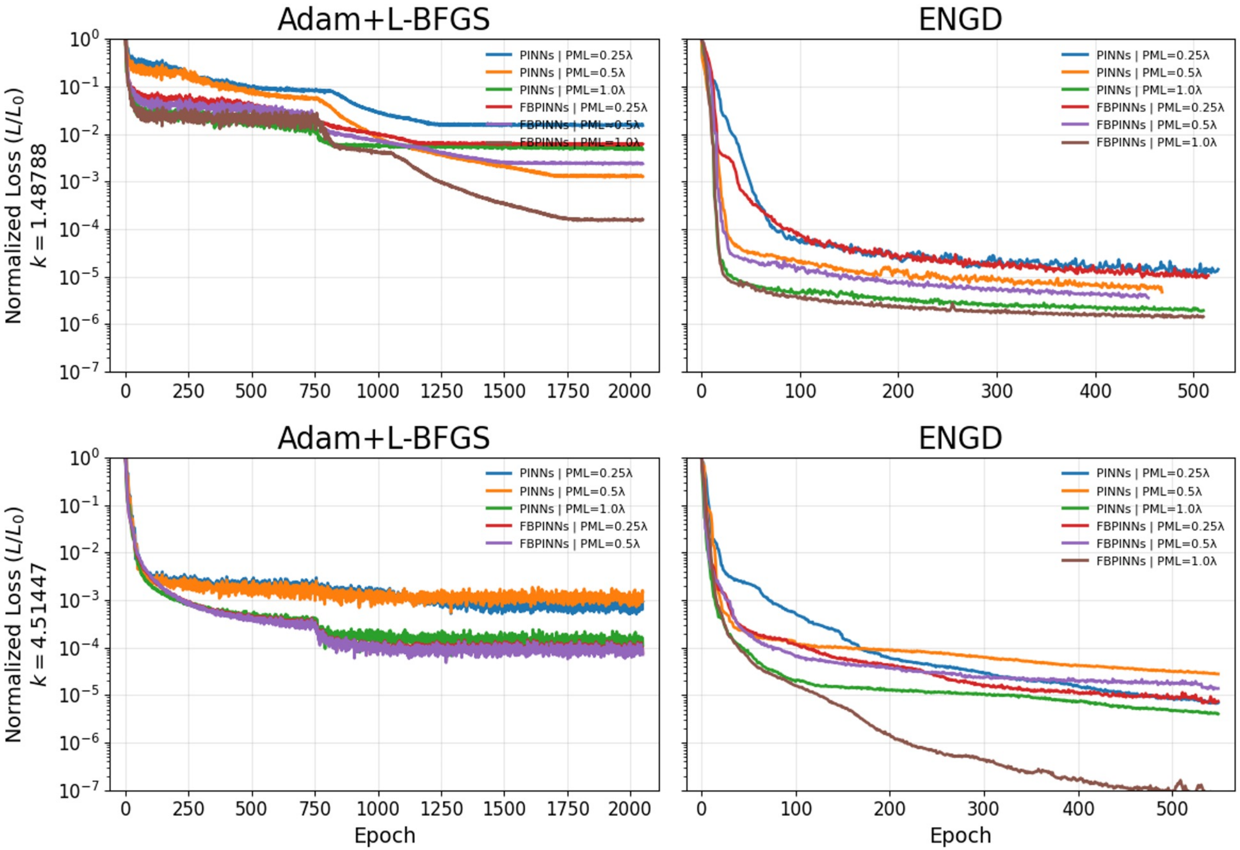
WP2 highlights

Multilevel distributed PINNs for frequency-domain acoustic problems



WP2 highlights

Multilevel distributed PINNs for frequency-domain acoustic problems



WP2 highlights

T2.1 – Surrogate models based on PINNs

Semi-Lagrangian neural methods for convection diffusion in large dimension

Key points

- Sequential in time neural based methods
- Transport of collocation points + projection on neural network space
- Natural Gradient optimizer + adaptive sampling
- Implemented in Scimba
- Characteristic approximation for diffusion

Results

- More accurate methods (compared to classical SL methods) after dimension 4
- Lower memory consumption

Dissemination

- Publication in CMAME, several presentations

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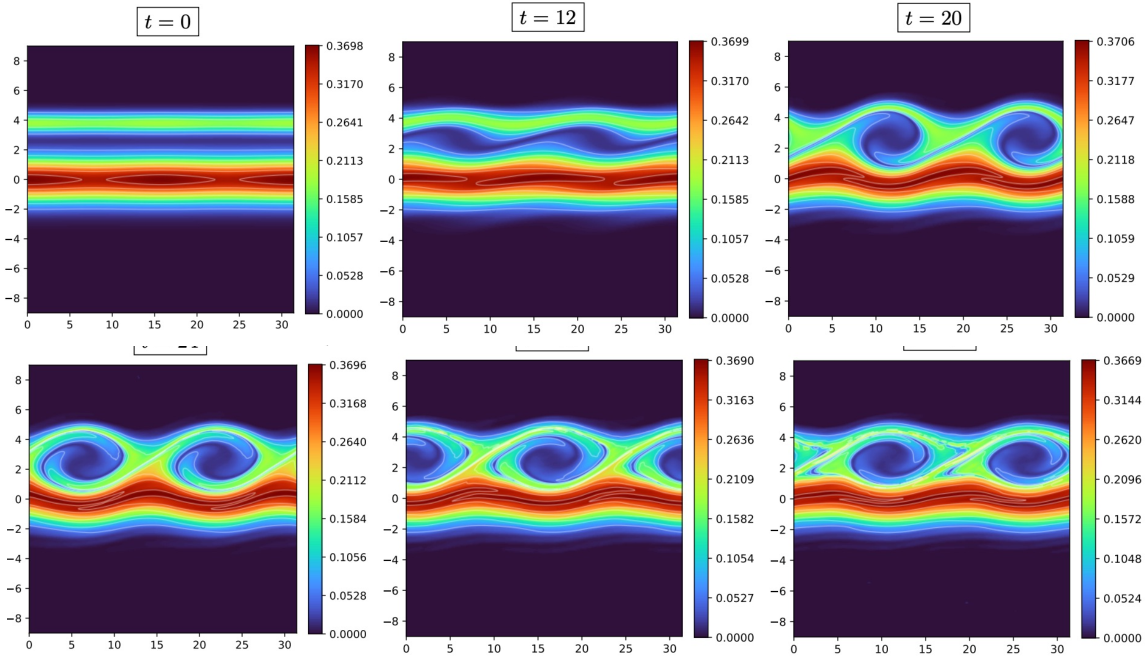
WP2 highlights

Semi-Lagrangian neural methods for Vlasov

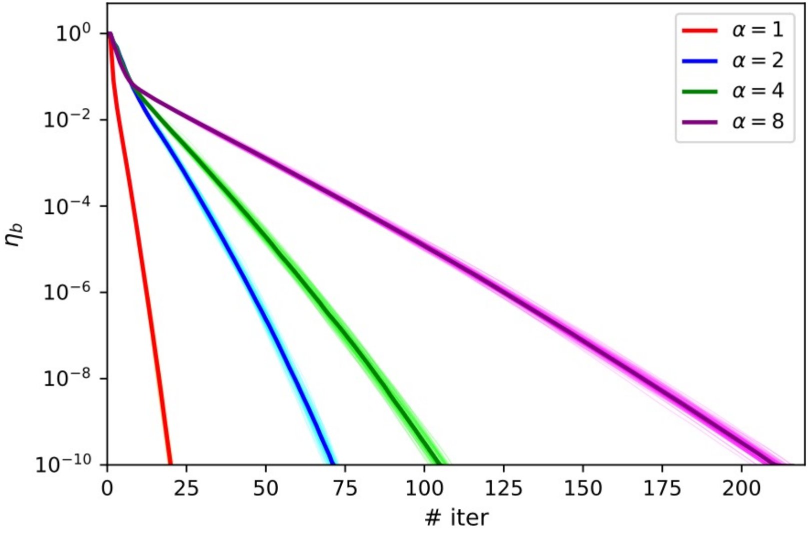


WP2 highlights

T2.2 - PDE operator learning with Neural Operators

Neural network for preconditioning

- Postdoc of Y. Xiang and M. Shpakovych (Inria – Airbus – Cerfacs @Concace)
- Solution of 2D Helmholtz equation with random velocity field, PML
- Trained neural network used as a preconditioner for FGMRES in mixed arithmetic



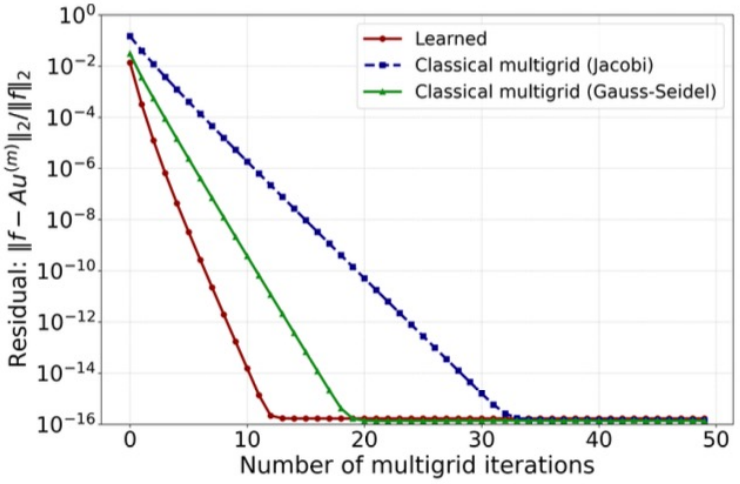
Generalization with respect to the size of the domain, learning performed with a=1

WP2 highlights

T2.2- PDE operator learning with Neural Operators
Learning to smooth: enhancing multigrid solvers with data

- Solution of 2D Poisson using geometric multigrid
- Trained Neural Networks used as smoothers in the multigrid solver

Pre and post-smoothers learned for N=64 (i.e., 64 x 64 mesh) : generalization capabilities on a 512 x 512 grid



(d) $N = 512$ and $L = 6$

WP2 highlights

T2.2 – PDE operator learning with Neural Operators
Neural operator coupled with classical code

Key points

- Fourier Neural operator to predict solutions of nonlinear elliptic PDE
- Classical scheme: FD + Newton-Krylov methods
- **Idea**: use the neural prediction as initial guess
- Full scheme is converged

Results

- CPU time gain 80-90% (close to divided by 2) on fine grids, and more on coarse grids
- On the considered benchmark, no situation of convergence fails

Dissemination

- Publication in Nonlinear simulation, several presentations

WP2 highlights

T2.3 – Data-driven model order reduction

Hybrid numerical methods for reduced modeling

Key points

- Work between Makutu@Inria and Macaron@Inria
- PINNs for parametric problem interesting but not accurate
- **Idea 1**: train parametric PINNs offline + enriching of FE basis with PINNs prediction
- **Idea 2:** online prediction on coarse grids since the basis is more expressive

Results

- For linear elliptic problem enrich FE allows to use mesh 3-4 coarser for same accuracy
- For 1000 parametric solutions solved we divide the full CPU time by 10 to 100

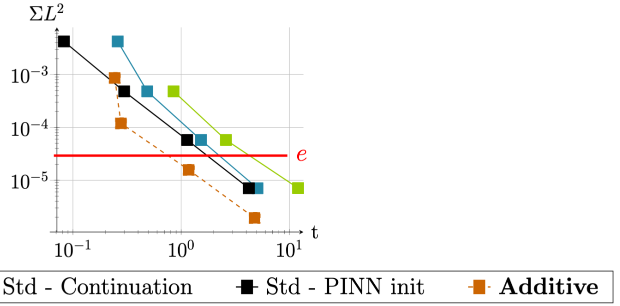
Dissemination

- Work submitted to M2AN, several presentations

WP2 highlights

Hybrid numerical methods for reduced modeling

$\boldsymbol{\mu}^{(2)} = (0.05, 0.05)$



N_{dofs} and execution time required to reach the same global L^2 relative error e :

Std vs Add	Number of DoFs		Execution times			
e	Std	Add	(nat)	(cont)	(PINN)	Add
$1 \cdot 10^{-3}$	7,828	2,748	0.58	0.39	0.19	0.24
$1 \cdot 10^{-4}$	35,884	14,623	1.95	1.14	0.8	0.32
$1 \cdot 10^{-5}$	167,583	70,303	9.39	4.16	3.4	1.59

$\div 2.4$ $\div 2$ $\div 2.5$ $\div 6$

WP2 highlights

T2.4 – Non-intrusive reduced basis methods for parametric problems
Nonlinear compressive reduced basis method

PhD thesis of Hassan Ballout (Université de Strasbourg)

Objective

- Mitigate the Kolmogorov barrier (for linear approximations)

Main assumption

- Only a few (first n) coefficients in a linear approximation are meaningful DoFs

$$u_{\boldsymbol{\mu}}^{n,N} = \sum_{i=1}^{n} \alpha_{i,\boldsymbol{\mu}} \varphi_i + \sum_{j=n+1}^{N} \psi^j(\alpha_{1,\boldsymbol{\mu}}, \ldots, \alpha_{n,\boldsymbol{\mu}}) \varphi_j,$$

Proposed methodology

- Linear encoder: projection on the first few modes
- Nonlinear decoder: involves a nonlinear model Ψ to predict the remaining coefficients

WP2 highlights
T2.4 – Non-intrusive reduced basis methods for parametric problems
Nonlinear compressive reduced basis method

Choice of n

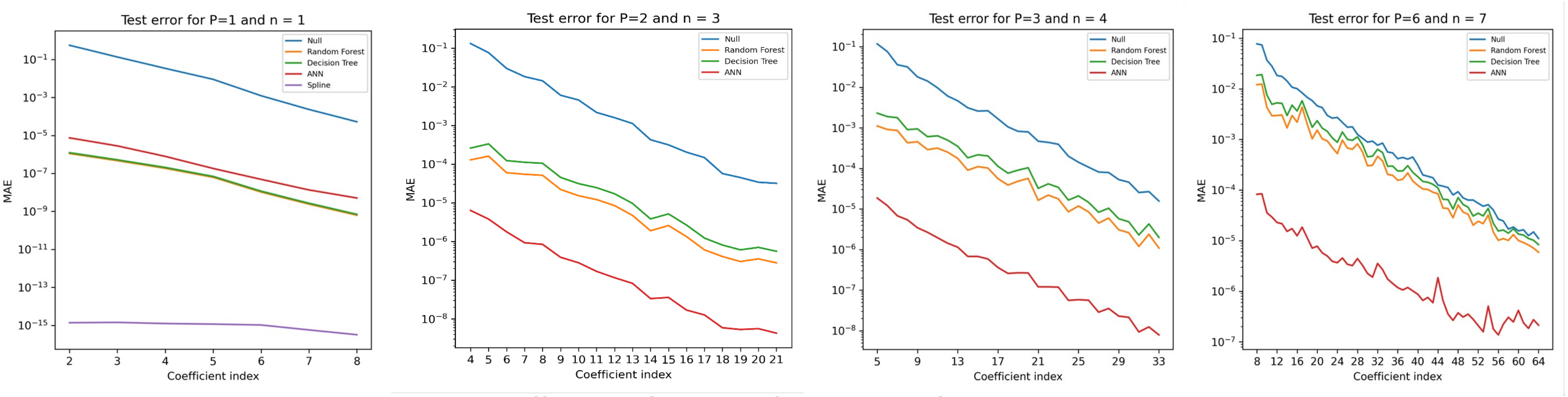
- Locally: n = p, where p is the number of parameters in parametric PDE
- Taylor + Davis-Kahan Matrix perturbation analysis - In preparation
- Globally: no upper bound, but in practice it is $n \gtrapprox p$

Improved version when the parameter is known

- Use it to predict the last coefficients
- Solve for the first ones
- This approach is more stable and preserves the linearity of the problem

WP2 highlights

T2.4 – Non-intrusive reduced basis methods for parametric problems
Nonlinear compressive reduced basis method



Predicting the N-n last coefficients from the first n ones for a linear elliptic problem

The choice of the nonlinear model is crucial for both accuracy and efficiency

3. WP2 future steps

WP2 Future steps

In relation with T2.1

- Multi GPU natural gradient + preconditioning for natural gradient
- Other efficient optimizers
- Adaptive sampling and optimal transport
- More efficient FBPINNs/MLFBPINNs and general geometry with domain decomposition
- More guarantees for PINNs
- Applications: waves and seismology, radiative transfer, plasmas for fusion, optical waves

In relation with T2.2

- Accurate neural operator for Helmholtz
- Structure preserving and invertible neural operator
- Neural operator for Maxwell
- New optimizers for neural operator + low rank/multi pole, approximation ?
- Work with unstructured meshes and GNNs / Transformers il linear system solvers

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