RESEARCH CENTRE

Inria Centre at Université de Lorraine

IN PARTNERSHIP WITH:

Université de Strasbourg, CNRS

2024

ACTIVITY REPORT

Project-Team

MACARON

MAChine leARning for Optimized Numerical methods

IN COLLABORATION WITH: Institut de recherche mathématique avancée (IRMA)

DOMAIN

Digital Health, Biology and Earth

THEME

Earth, Environmental and Energy Sciences

Inria

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Project-Team MACARON

Creation of the Project-Team: 2024 April 01

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2 Overall objectives

Many applications in physics and biology require the numerical resolution of complex nonlinear and/or multi-scale Partial Differential Equations (PDEs). In general, for these problems, classical numerical methods hardly guarantee stability and accuracy. A typical example is the resolution of the compressible Euler system for fluid flows. This non-linear model produces discontinuous solutions and thus high-order accurate methods require sophisticated empirical stabilization procedures to avoid spurious Gibbs oscillations. Additionally, in the nearly incompressible regime, when the acoustic waves of the Euler system propagate very fast, the classical schemes have to satisfy very stiff constraints on the discretization parameter to be stable and accurate.

To design appropriate numerical schemes with both stability and accuracy properties, an essential point is to preserve the properties of the physical model at the discrete level. For over twenty years, the CALVI project-team, followed by the TONUS project-team, have proposed such numerical methods whose main applications include plasma physics and compressible fluid mechanics.

These methods have often been able to solve difficult problems, with reduced computational cost compared to standard approaches, and team members have become increasingly proficient in the numerical methods for multiscale hyperbolic and kinetic equations.

Examples include relaxation methods for implicit hyperbolic PDEs, asymptotic preserving and well-balanced schemes for conservation laws with source terms [91, 92, 73], or moment methods [67] and semi-Lagrangian schemes [86] for multi-scale kinetic PDEs.

However, most of these methods require a suitable choice of parameter values (relaxation schemes [76, 60, 43], splitting coefficients, artificial viscosity [97], slope limiters). These choices often depend on the target solution itself. During the existence of CALVI and TONUS, we have also tried to propose reduced models based on general moment and water-bag approaches, or asymptotic approaches. These techniques have also shown some limitations in terms of saving computation time. The limitations that the team has noted in recent years in the use of traditional methods have led us to consider very different techniques.

In the meantime, machine learning (ML) methods have made tremendous progress. In 2012, the impressive results obtained by the AlexNet neural network [65] for image classification convinced several scientific communities that neural networks would be a central tool in the estimation of functions in large dimension by supervised approaches. Since 2015, deep reinforcement learning approaches have also achieved spectacular results for game strategies in chess and Go [85, 74]. This has opened up new opportunities to continuously optimize systems while using them. In view of these major advances in deep learning, the scientific computing communities have already seized upon these tools for several purposes:

- the construction of numerical methods assisted by neural networks [83, 81],
- the construction of reduced models [63, 51],
- the creation of neural network solvers for PDEs [80] or the training of neural networks to solve inverse problems [49, 89].

In this project, we want to study and design numerical methods enriched by deep learning, in order to gain efficiency in solving direct and inverse multiscale and nonlinear problems. More precisely, we aim at reducing the computational time and memory consumption to obtain the solution at a given precision: this could be achieved by increasing the accuracy of the method tuning some part of the scheme or using some fast prediction obtained by ML approach. Another way will be to use reduced models to speed up the simulations.

For this purpose, we elect to use supervised methods as well as reinforcement learning (RL) approaches, which can be interpreted as a combination of deep learning and optimal control.

In the case of numerical methods, a first approach consists in learning the optimal parameters of the method using samples of numerical solutions obtained with different parameters. Another one, called differentiable physics in the literature, is to express the whole numerical scheme as the composition of classical functions and neural networks and optimize it with the gradient descent algorithm and automatic differentiation.

This enables us to learn a part of the scheme using the results produced by the whole simulation. The differentiable physics approach seems to be easier to train but it is an intrusive method since one has to write the scheme in frameworks like `PyTorch` or `TensorFlow`. The RL-based approach seems more difficult to implement and train but is non-intrusive.

Finally, solving inverse problems may be tackled by constructing reduced models with neural networks and then applying classical optimization algorithms on a small dimensional problem. One difficulty is to ensure the generalization of the neural networks, i.e. their accuracy when applied to data not processed in the learning phase. For this, the training data must be diverse, realistic and numerous. These require the development of highly efficient and accurate solvers, as well as suitable neural network architectures and training schemes.

Classical PDE solvers, such as finite volume, finite elements or reduced order modeling, are extensively used in industrial and scientific applications because they ensure convergence and stability, as well as the conservation of certain physical properties. For the **data-driven solvers and models** we wish to develop, the central issue is to improve the efficiency of the methods while preserving the mathematical guarantees provided by the numerical analysis. This will be a key criterion in the following research program, dedicated to the resolution of direct, inverse and control problems.

To ensure such guarantees on the numerical solution, we focus more on integrating ML in the solvers, rather than on improving ML methods by using physical or numerical priors. However, our research may lead to developing new network architectures or new learning methods, even if this will not be its central element.

3 Research program

3.1 Data-Driven Solvers

In this research axis, we plan to investigate data-driven solvers to obtain more accurate and less time-demanding numerical simulations. Classical numerical methods have important guarantees like convergence, stability or structure preservation like divergence free constrains, which are essential in most applications. A key aspect of our research is to ensure the same properties even when ML is used to supplement the numerical methods. To complete this axis, we explore three different approaches:

1. optimize parts of numerical solvers,
2. optimize the representation of the approximate solutions,
3. include data-driven predictions of solutions to accelerate numerical methods.

3.1.1 Optimizing parts of numerical solvers

High fidelity simulation of compressible fluids still remains an important challenge, and we are convinced that solving it would benefit from recent deep learning tools to optimize space and time discretizations, among which the Finite Volume, Discontinuous Galerkin or Lattice Boltzmann methods. For nonlinear problems such as the Euler system or the shallow water equations, theory has been developed to ensure that the numerical schemes capture the right solution. However, this theoretical framework does not always indicate how to adapt the schemes, especially high-order schemes that admit numerical instability problems, to increase accuracy or preserve certain physical properties. Choices are then sometimes made in a heuristic way by tuning some parameters in the schemes:

- numerical Finite Volumes flux corrections and slope limiters [77],
- artificial viscosity for Discontinuous Galerkin schemes [46],
- relaxation matrix/equilibrium function for multi-scale relaxation schemes and the Lattice Boltzman Method [71],
- well-balanced corrections [73, 50].

These choices could be greatly improved using machine learning techniques. Our aim is to design these key parameters automatically. This will simplify the use of these schemes (because the parameters will no longer have to be chosen by the user) and increase the accuracy of the methods (because the parameters will be chosen in a more optimal way). These strategies are particularly well-suited to high-order schemes, where the extra precision is offset by lower stability, which is often subject to correction. For that, we will consider numerical neural networks but also symbolic regression methods which make it possible to obtain analytical formulas.
The team has specialised in schemes based on relaxation approaches before avoiding or limiting the restriction of the CFL condition. These include the kinetic relaxation approach [11, 43, 47] and the Xin-Jin/Suliciu relaxation approaches for multiscale problems [91, 93]. We will continue developing these approaches, in particular by extending them to more difficult problems and increasing the order of accuracy. The numerical methods thus obtained are then to be coupled with machine learning to make them more effective.

One of the main challenges is to incorporate these data-driven functions into the schemes, while still preserving the classical properties of the schemes: convergence, stability, entropy dissipation, positivity of the solutions, etc. To achieve this, the exact data-driven function, as well as the training procedure, must be chosen carefully. More precisely, the choice of the so-called loss function, which is optimized in the learning steps, is crucial. We will explore supervised learning where loss functions compare the learned function to reference ones, as well as unsupervised learning, where the loss functions do not refer to any reference functions, e.g., residual loss functions in PINNs (Physics-Informed Neural Networks [80]) or discriminative loss functions that can detect defects in classical schemes (Generative Adversarial Networks [53]).

The structural method for hyperbolic systems: optimisation with machine learning. One of our focuses will be on structural methods. In recent years, these methods have been introduced to build very high-order numerical schemes to solve PDE on compact stencils [42]. A particularity of this finite difference method is that it not only approximates the PDE solution with high order accuracy, but also its derivatives. It relies on defining two independent sets of discrete equations, the physical and the structural equations. The physical equations describe the physics of the problem, i.e. the underlying PDEs. As such, treating problems with specific constraints (for instance, ensuring that some vector field is divergence-free) becomes a matter of adding or modifying a physical equation. The structural equations are responsible for the order of the discretization, and thus their modification makes it possible to treat non-smooth solutions or improve the accuracy on continuous ones.

The overarching goal of this axis is to extend the structural method to hyperbolic systems with source terms, in at least two space dimensions, for applications in e.g., fluid mechanics or electromagnetism. The structural method is well-suited to such systems, since the separation between physics and discretization provides a natural setting to construct schemes adapted to the situation under consideration. To that end, we want to construct a scheme that can switch on or off physical and/or structural equations locally and on the fly, depending on the properties of the solution (regularity, wave speeds, etc.), resulting in problem-adapted schemes. Moreover, operating this switch with machine learning techniques could make the adaptation parameter-free and more efficient.

Applications. The optimized methods will first be tested on simple equations. They will then be implemented on multi-physics systems, where they will allow a more important gain. We will consider Magneto Hydro Dynamics equations (MHD, coupling plasma dynamics and electromagnetism) and general Symmetric Hyperbolic Thermodynamically Compatible models (SHTC) [52]. The SHTC model constitutes a monolithic mathematical framework that encompasses the evolution of all considered materials and provides a unified mathematical description of multi-physics systems. See e.g. [82] for a generalization of the two-phase flow model to an arbitrary number of phases. Consequently, for these applications, we also need to design new schemes that are well suited for capturing asymptotic limits or steady states with stability guarantees before thinking about hybridization. For systems like MHD or SHTC, such schemes do not exist at the moment. To develop them, we shall focus on semi-implicit relaxation schemes and reference solution schemes, for which machine learning optimization is well adapted.

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3.1.2 Meshless and neural approaches

PINNs and Neural Galerkin approaches. Physics-informed Neural networks [80, 94] and Neural Galerkin [37, 48] are two recent numerical methods to solve PDEs. Contrary to classical approaches, these methods use nonlinear (compared to the degree of freedom) finite-dimensional functions, like neural networks, to represent the solutions to the PDE. These methods have two main advantages compared to classical ones: they are able to deal with large-dimensional problems and are mesh free, but they suffer from a significant lack of precision in certain applications. However, they remain interesting for some applications or coupled with conventional methods. We therefore wish to study such approaches, moving in particular towards architectures and training that are more specific to the PDEs considered in the team (mainly kinetic equations and hyperbolic PDEs), and which preserve some properties and structures of these problems. These new methods can be used directly, like solvers, or coupled with classical methods as explained in the next sections.

Neural operator approaches. Neural operators [64] are new tools which make it is possible to construct a map between functions approximating the inverse operator of the PDE. The resulting network can be interpreted as a surrogate model of the PDE. Most common are Fourier Neural operators [68] (and their Physics-informed version [69])) and DeepONets. There is currently a lot of work being done on these networks. In our context, we would like to develop mesh-independent or continuous approaches (such as those based on neural implicit representations [84, 78]), which are capable of dealing with multi-scale and hyperbolic problems. This results in networks that are more specific to a given PDE in order to preserve its essential structures. Theoretical tools such as Green's functions [34], Duhamel's formulae, particular solution profiles or asymptotic developments can be used.

Super-resolution. Signal-processing and learning-based super-resolution techniques will also be leveraged to tackle forward and inverse problems connected to the wave equation with boundary conditions, e.g., *hearing the shape of a room* [88]. Indeed, these equations can be well approximated by geometric approaches [31] or by the method of fundamental solutions [66]. These amount to replacing boundary conditions with source terms that are sparse measures, e.g., mixtures of Dirac measures. Recent methodologies enable the meshless recovery of such sparse measures through optimization schemes [45] that could lend themselves well to hybridization with deep learning, as outlined in Section 3.1.4.

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3.1.3 Optimizing the representation of the approximate solutions

Neural network basis functions. Some numerical methods, like the Discontinuous Galerkin and Finite Element methods, are based on a representation of the numerical function in a spatial basis. The idea is to construct better basis functions in some parameter regimes that are well-adapted to the target solutions. This will increase the accuracy of the methods, while retaining crucial convergence and stability properties. Preliminary results are encouraging.

A first possible way to proceed is to compute neural network predictions of solutions with the PINNs or neural operator methods developed and studied by the team to learn some set of coarse solutions and insert them into the basis representation. This will require some works on the architecture and the training of the neural networks. First tests would be done on elliptic equations with FE and then the method will be extended to steady state solutions of hyperbolic equations with Discontinuous Galerkin methods. Longer term goals include the resolution of time evolution problems with space-time Discontinuous Galerkin methods, as well as transport equations with semi-Lagrangian solvers [86]. Another interesting point would be the extension of this data-driven method to structure preserving FE methods, that preserves the geometric structure of the equations [32].

A second way to proceed consists in determining the basis functions using the so-called differentiable physics method: the approximate solution obtained with the FE or DG scheme is written as a global function including neural network basis functions and then the approximation error is minimized by using gradient descent. This requires that the whole scheme can be written as a differentiable function. This could correct specific drawbacks of classical bases, which trigger numerical pollution when the flow regime is dominated by convection.

For the two approaches, it will be important to prove that, under some reasonable conditions, the data-driven methods still converge and possess some stability estimates.

Neural network predictions in PIC methods. The Particle in Cell method is used to simulate the time evolution of ions and electrons interacting with electromagnetic fields. The principle is to approximate the distribution of physical particles by macro particles, each representing thousands of physical particles. The macro particle dynamics is obtained by solving Maxwell's equations on a mesh grid with a Finite Element solver. The PIC method works independently of the dimension, but it converges slowly when increasing the number of macro particles and tends to be plagued with numerical noise. To obtain a better accuracy, one can reduce variance [87] when estimating integrals like density or current. We consider the same approach as above to improve the accuracy by incorporating some local prediction of the solutions.

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3.1.4 Including data-driven predictions into numerical methods

Iterative methods optimized by deep learning. In the PDE world, many problems boil down to applying some iterative algorithm: for instance, iterative solvers for linear inversion, the Newton method for nonlinear inversion, or optimal-control-based methods for inverse problems. Here, we propose to design tools, based on neural networks, to accelerate the convergence of the original iterative method. For the Newton method and inverse problems, we elect to train neural networks to give an approximation of the solution, and to use this prediction as the initial guess of the iterative method. This approach has two main advantages: first, if the training fails on some data and does not give a good prediction of the solution, the convergence will be as slow as without neural networks, but the problem is still correctly solved. Second, since the final solution is given by a numerical method, all the properties of the numerical scheme will be conserved. Here, the artificial neural network can be merely viewed as a predictor step. For this type of application, we can use convolutional neural networks, graph neural networks [36], or mainly neural operators [64], mentioned in the previous section. Indeed, in this case the same operator could be applied to any mesh and numerical method. For matrix inversion, the idea will also be to predict the inverse of the system using a neural network. This predictive algorithm could be seen as a right preconditioner. However, since the convergence depends on the spectral properties of the preconditioned system, imposing additional constraints during training might be necessary. In this case, the input of the network will be a matrix, and it will be essential to find a good network architecture for this problem. Graph convolutional neural networks [35], which take adjacency matrices as inputs, would be a possible choice. When a linear system with a specific structures needs to be inverted, faster and parallelizable iteration schemes, such as the alternate direction method of multipliers (ADMM), can be unrolled into deep neural networks and further optimized, as reviewed in, e.g., [70].

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3.2 Self-specialization of numerical solvers

The goal of the first axis is to develop new numerical methods assisted by neural networks in order to increase their efficiency. For this purpose, we need to pre-train the networks on a set of simulation data. With neural networks of reasonable size, it seems unrealistic to do it efficiently on all possible physical configurations (initial data, parameters, geometries), even related to a single equation. In general, in a group of users, the code will be used in a much smaller set of configurations. Therefore it seems more natural that learning is specialized to the simulations of each user. We will study strategies to automatically adapt the methods developed previously to the simulations performed by the user so that he/she does not have to manage the training. We call this process the self-specialization of codes. The works of this subsection is a priority for the team, but will be carried out in the **medium to long term** once our expertise in hybrid models is greater.

3.2.1 Continual learning, sampling and likelihood

To obtain robust code that learns from the data produced by the code, we need to use continuous learning methods (data that arrives regularly) and to detect if the code is going to be used in a configuration where the neural network is not going to work in order to de-activate the network, for example. The second problem in learning is the detection of out-of-distribution examples (OOD) [95]. We propose to study different methods for that and apply them to our hybrid simulation codes. We could use generative models (Variational auto-encoders [61], normalizing flows [62], Denoising Diffusion Probabilistic Model [58]) in order to capture the probabilistic distribution of the inputs data of the code. This will allow us to test whether a new input has been produced by the distribution. If this is not the case, the network is likely to fail. Another important problem is to make the training *continuous* while a given simulation code is used, in order to become specialized to the data given by the user. We can model the parameters and initial state space S_0 by a time-dependent probability distribution where the evolution is assumed to be smooth over time. The aim will be to develop learning procedures that can capture p_t using a large training set at $t = 0$ and smaller data sets at later times $(t_1, ..., t_n)$, in order to limit data storage requirements. These small sets of continuously arriving data correspond to the data produced each time the code is used to produce a simulation. This type of approaches are referred to as continual learning or life-long learning in the literature [59]. Their use in the context of PDEs has not been explored, to the best of our knowledge. Continual learning could be used on all the supervised models developed in our project team, or specifically on generative models that could in turn be used to train other neural networks by means of generating examples following the relevant distribution.

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3.2.2 Self-specialized numerical methods

Combining the data-driven solvers from the first axis with continual learning and Out-Of-Distribution Detection approaches, we wish to design complete prototypes of self-specialized codes. In practice, we would like to validate this approach for two particular numerical methods in simple configurations.

First use case: we construct a 2D or 3D Lattice Boltzmann scheme code for Euler, MHD or SHTC equations with some guarantees on the stability of all regimes. We will use a general relaxation matrix (multiple relaxation time method). Using a reinforcement method or the differentiable physical approach, we will learn the relaxation matrix such that the discrete residue or the error compared to a fine solution computed by the user will be minimal. To obtain a full prototype we must add a mechanism for continual learning and a mechanism of OOD detection. We must also include a safety mode of the method in this case.

Second use case: we write a hybrid finite element code for implicit time integration for strongly nonlinear equations (nonlinear anisotropic diffusion, reduced MHD). The idea will be to construct a first approximation of the solution using a parametric PINNs or a Neural operator (like Fourier Neural Operator) and integrate this approximation inside the numerical methods. This approach will be used to enhance the basis functions and accelerate the Newton convergence. One of the main questions is how to construct the learning process with data which arrive step by step. We consider an implicit scheme with a Newton method (neural networks which take data and previous time step input) with adaptive time step. If the Newton convergence is fast, we increase the time step at the following step. If there is no convergence, we recompute the time step with a smaller Δt. The more we make simulations, the more we collect data to increase the accuracy of the neural network for the prediction of Newton's method.

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3.3 Data-driven modeling

In order to reduce the computational cost of simulations and to move towards real time simulations, there is a lot of research into the construction of reduced models. We can mention classical approaches such as moment models or reduced basis methods (order reduction). The development of machine learning methods offers new opportunities to build these models, especially in highly nonlinear regimes. We wish to investigate several ideas on this topic.

3.3.1 Reduced models in asymptotic regimes

In some previous and ongoing works (ANR MILK), we have studied the construction of reduced models for kinetic equations in different asymptotic regimes using neural networks. Such reduced models are very interesting since kinetic equations describe the evolution of distribution in phase space (position-velocity), their full numerical resolution would require a lot of computing resources and thus reduced models are much cheaper to simulate. We consider two different types of asymptotic regimes.

The first asymptotic regime is the collisional regime. When the collision rate is high, the velocity distribution function tends to be Gaussian and analytical reduced models are well known: these are the Euler or Navier-Stokes systems. However, for weakly collisional regimes, there are no such analytical reduced models and this is where neural network can help. We have started a work on the non-local closure problem of the Euler equations for the Vlasov-Poisson dynamics [54, 33] and we would like to generalize it to more complex physical problems: complex collisional operator, two species coupling, Vlasov-Maxwell dynamics with method able to be invariant to the spatial grid and potentially interpretable. We can also consider generalized moment models [79, 55] and aim for a network to learn the choice of moment and the local closure. In this context, we propose to ensure the entropy stability of the models obtained since local models are easier to study. This type of method will also be used to design macroscopic biological models using particle simulations (ANR Mapeflu). The company AxesSim is very interested in Vlasov-Maxwell simulations and has optimized codes for hyperbolic equations. The construction of reduced models within this framework would be an important axis of collaboration.

The second asymptotic regime is the strong magnetic field regime. Indeed, in this regime, the charged particles will rotate rapidly around a slow trajectory. Since following the highly oscillating trajectories would be very computationally demanding, we would like a model for the slow trajectory only. In sophisticated physical configurations (e.g., for non-periodic magnetic fields), deriving an analytical solution is difficult if not impossible. Using neural networks, we would like to filter the fast oscillating dynamics and then devise a reduced model. In addition, separately reconstructing the fast rotation dynamics would make it possible to add relevant corrections to the slow dynamics model. This would allow us to construct valid schemes in different magnetic field magnitude regimes [44].

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3.3.2 Continuous Reduced Order Modeling (CROM) for strongly nonlinear PDEs and kinetic equations

The Reduced Order Modeling (ROM) and reduced basis methods [56] have demonstrated their powerful capabilities for many problems. They are based on a “projection" of the model onto a reduced basis obtained by singular value decomposition of snapshots of the solutions [41]. However, they have difficulties in reducing hyperbolic PDE dynamics and highly nonlinear problems. Since some years the main alternative is based on auto-encoder neural networks [72, 63]. Imposing a symplectic structure in these methods is part of the ANR project MILK, where we investigate reduction with manifold learning or auto-encoder approaches. In this project, we propose to focus on a very recent approach called **Continuous ROM** [40, 39, 96], which is based on the **implicit neural representation paradigm**. The classical ROM approach discretizes the PDE to obtain a large dimensional ODE and compresses this ODE with a Convolutional Auto-encoder or POD. Here, the idea to represent the solution (decoder) using a MLP coordinate based network which depends also on latent variables which are obtained by an auto-encoder. As in the ROM approach, the aim is to write the dynamics on the latent variable. All the works on physics-informed neural networks will be used for the decoder. For the encoder process, we will investigate some permutation-invariant neural networks or greedy approaches. Here, we propose to study multiple strategies to learn the reduced model (Reduced Galerkin projection, differentiable physics learning, classical supervised methods). We will also study how to incorporate the properties of the PDE in these reduced models (asymptotic limits, well-balancing, symplectic properties, Poisson brackets [57] or entropy dissipation, which is essential for stability). We will mainly apply these news approaches on nonlinear conservation laws, wave equations and kinetic models. These approaches could also be interesting to compute a reduced basis only in the velocity space for kinetic equations. To obtain explicable and easy to disseminate reduced models, we will couple these methodologies with symbolic regression methods (see e.g. [90, 38]) which allows to learn analytic formula. Comparing to the classical approaches, the reduced models obtained with CROM approach can be used on any meshes and consequently coupled with any code without additional interpolation step and can be used with symbolic approaches. Obtaining analytical models is not possible with traditional ROM approaches.

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3.4 Data-driven optimal control and inverse problems

While the previous axis focused on improving numerical methods using recent deep learning methodologies, this axis focuses on improving optimal control algorithms and the resolution of inverse problems, where we solve many forward problems (subsection 3.1) and use reduced models (subsection 3.2), using deep learning approaches.

3.4.1 Reinforcement Learning methods for PDEs and high dimensional action spaces

In the last decade, many RL algorithms have been written by the machine learning community. This approach allows constructing feedback loops that are essential for real-time control. Some of these methods can handle a continuous action (control) space. However these methods are more difficult to use in large-dimensional action spaces and for long time problem. Indeed, depending on the application, there may be problems with exploration (we do not know the action space correctly) or with precision and regularity (it is more difficult to obtain precise control compared to classical gradient approaches). For such problems, the control is a spatial function (discretized in general) so the dimension is large. In this case we are not able to correctly define an admissible/realistic action and sample the action space. For this reason, these algorithms generally make use of a basic parametrization of the action function which is very restrictive. We propose to use generative models/operators to construct probabilistic policies able to explore large-dimensional structured actions, and to couple this with gradient methods (adjoint approach, PINNs) to guide the exploration towards interesting areas. These methods will be an alternative to differential physics to train large networks (which is a very costly, and sometimes unstable, approach) present in numerical schemes or physical model taking into account of the long time stability.

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3.4.2 Optimal control and physics-informed ML

Recent work, such as [75] have used PINNs to solve open loop optimal control problems. These methods could be very interesting for solving high dimensional problems, closed loop problems, or shape optimization, which is equivalent to a neural implicit representation. Indeed, for closed loop problems, standard approaches based on the Hamilton Jacobi Bellman equation are very cumbersome to implement. We will study these methods from a theoretical point of view on simple cases and their practical improvement. We will also investigate the extension of these approaches with physics-informed neural operators, which seem to have a greater approximation capacity than PINNs and could be efficient to treat inverse problems in high dimension. Another strategy we propose is to use generative models. Generative models, like diffusion models, make it possible to sample high-dimensional probability distributions. Recently, a new approach to robot control has been proposed. It consists in training a diffusion model to build an efficient control from a random control. This amounts to concentrating a probability law of controls on the most optimal control using physics-informed loss. We propose to couple this with Neural encoder approaches and apply it to control PDEs and inverse problems.

Team members involved: *C. Courtès, A. Deleforge, E. Franck, V. Michel-Dansac*

3.4.3 Accelerated open loop optimal control by ML

Optimal control methods that are based on the Pontryagin maximum principle and gradient-based methods are very computationally intensive. Reducing the computational cost of these methods is an important issue, that could be solved using machine learning. In a similar way to the case of Newton's method, Neural operator/PINNs approaches can be used to obtain an approximate solution of the control problem which will be used as an initial guess to accelerate the convergence of the iterative methods. We will also study another approach which consists of using reduced modeling to accelerate each step of the gradient method. We have recently constructed a method where we control a complex problem by constructing a reduced model which is checked and corrected according to the effect of the control obtained on the full model. We wish to focus on correcting the reduced model (which may be invalid in some areas) as the control algorithm proceeds. These approaches could be viewed as model-based Reinforcement learning and will use our work on reduced modeling in Section 3.3. This project is a lower priority than the other optimal control projects.

Team members involved: *C. Courtès, A. Deleforge, L. Navoret*

3.4.4 Inverse problem and super-resolution

We consider the following inverse problem: given a discrete-time measurement of the propagation of a sound impulse from a pointwise, omnidirectional source to a microphone array (called RIR or Room Impulse Response), can we estimate the geometry of the room? As part of Tom Sprunck's PhD, which started on November 1, 2021, this question has been partially addressed theoretically and numerically, in the case of cuboid rooms. To formalize this problem and deal with numerical aspects, we are investigating the use of the so-called image source method, that allows replacing the boundary of the room to be reconstructed by a constellation of image sources corresponding to iteratively reflected copies of the original sound source with respect to the walls of the room. The question can then be formulated as an optimization problem which consists of identifying the positions of a linear combination of Dirac masses in space — the image sources — from discrete time observations of the solution of the wave equation at the microphones (the RIRs), which are imaged by a linear operator. Knowing the positions of the image sources up to order 1 is then sufficient to reconstruct the geometry of the room. This problem is thus part of the recent framework of super-resolution, which aims at reconstructing the positions and amplitudes of the peaks of a sparse measurement from linear observations. We consider here a convex relaxation of the problem by extending it to the set of Radon measurements (BLASSO). We are currently considering the implementation of efficient numerical methods exploiting this relaxation. To make the method applicable to real world data that feature complex frequency- and angle-dependent responses of sources, microphones and reflecting surfaces inside the room, we intend to hybridize these methods with data driven techniques. These could be achieved by training generative models on real databases of source, microphone and wall responses, or by using *deep unrolling* on parts of the optimization scheme, in order to optimize them end-to-end on real or realistically simulated data.

Team members involved: *A. Deleforge, E. Franck, L. Navoret*

4 Application domains

The objective of the project is to design new numerical methods and reduced models by leveraging machine learning. The team is focused on three main applications.

Plasma modeling for nuclear fusion. To design future devices (stellarators or the DEMO Tokamak), physicists need numerous parametric studies in various physical flow regimes. Since the simulations involving MHD or Vlasov-type equations are extremely computationally costly and use a large number of degrees of freedom, it is necessary to design reduced models or cheap numerical methods to run these parametric studies. We collaborate with CEA Cadarache and the Max Planck Institute for Plasma Physics to build reduced models and solvers (PIC method, FE method) enriched by machine learning to quickly solve parametric models in well-defined configurations in real time or on simple laptop. Discussions have also started with some colleagues from the Culham Center for fusion. A goal of this work is to propose neural methods applicable in this context, with a subsequent transfer to physicists. In the longer term, such reduced models could also be used in the context of real-time control of future devices. Together with our collaborators, we wish to position ourselves on this issue, which will become central for the integration in reactors and experimental devices. Physicists also need intermediate models, between microscopic kinetic descriptions and macroscopic fluid flows, to accelerate simulations in intermediate regimes. This framework is perfectly suited for the development of our closure and moment models. This work would also be of interest to astrophysicists working on plasma physics, and we plan to collaborate on these problems with researchers from the Strasbourg Observatory. In addition to the challenge of reducing computing times, the design of reduced models that can be interpreted using symbolic regression methods would enable physicists to better understand and study the link between certain quantities and phenomena.

Compressible multiphase flows – energy applications. Some of our work on numerical schemes coupled with learning and reduced modeling focuses on compressible and multiphase fluid mechanics models. Such equations have a huge range of applications. Among them, we wish to focus on modeling and solving gas-liquid interactions in thermal power plants. In particular, we collaborate with EDF (French electric utility company) on the construction of numerical schemes, as well as on the modeling of pressure laws, for its pressurised water reactors. In this context, we also wish to accelerate numerical codes in order to carry out large parametric studies for new design and real-time command, while being able to certify the result, given how critical this application is.

Inverse problems in acoustics. The last application is inverse problems in acoustics. The goal is to reconstruct the propagation medium of an acoustic wave from partial, discrete, band-limited or noisy measurements of the same wave, e.g., with microphones. A main focus will be on inverse problems in building acoustics, and in particular on automated acoustic diagnosis. These inverse problems are particularly challenging for two reasons. Firstly, they are highly ill-posed and hence require the careful use of model- or data-driven regularizers. Second, an exhaustive modeling of all acoustical phenomena occurring in real world data is impossible, which requires a strong robustness and adaptability of the devised methods to model mismatch. These challenges will be tackled through the development and hybridisation of accurate numerical solvers for the wave equation, PDE-type optimal control methods, as well as approaches closer to signal processing and machine learning. The proximity with the UMRAE research at CEREMA Strasbourg, specialized in environmental and building acoustics, has made it a natural collaboration for several years. A long-term objective is to build new acoustic diagnostic tools for acoustic engineers and technicians. The numerical methods developed for this application could also be used for inverse acoustic problems in seismology, and we will also interact with the MAKUTU Inria team (Pau), whose work involves such problems.

5 Social and environmental responsibility

5.1 Footprint of research activities

The main environmental footprint of MACARON is likely due to travels to international conferences with airplane, which have been kept to a reasonnable amount per team member this year (strictly less than one on average). While the footprint of large scale computation could also be a factor, the scale of compute used in MACARON at this stage is negligible in comparison to, e.g., the training of large generative models.

Since the dissolution of the local commision on sustainable development (CLDD) of Inria Nancy, A. Deleforge is representing Inria Nancy at the regular national meetings gathering the CLDD representatives of all national Inria centers. A meeting between Bruno Sportisse and these representatives was organised in September 2024 to discuss the positioning of Inria with respect to the environmental footprint of both research acitivities and results, and a number of mid-term objectives were outlined.

5.2 Impact of research results

The research results obtained by MACARON this year and listed in this report do not have any obvious bearing, positive or negative, on environmental or social issues.

6 New software, platforms, open data

6.1 New software

6.1.1 acoustic-sfw

Name: Hearing the Shape of a Shoebox Room

Keywords: Acoustic Model, Acoustics, Inverse problem, Super-resolution

Functional Description: 1) An adaptation of the Sliding Frank-Wolfe algorithm for the gridless 3D recovery of image sources from room impulse responses recorded with a compact microphone array. The algorithm is described in details in this article: [1] Sprunck, T., Deleforge, A., Privat, Y., & Foy, C. (2022). Gridless 3d recovery of image sources from room impulse responses. IEEE Signal Processing Letters, 29, 2427-2431. HAL: https://inria.hal.science/hal-03763838/

2) An algorithms that recovers the 18 input parameters of the shoebox image source method from given such an estimated image source point cloud, namely: - The room's width, depth and height - The 6 DoF room translation and rotation in the array's coordinate frames - The 3D source position - One absorption coefficient for each of the room boundary.

The algorithm is described in details in this article: [2] Sprunck, T., Deleforge, A., Privat, Y., & Foy, C. (2025). Fully reversing the shoebox image source method: From impulse responses to room parameters. IEEE Transactions on Audio, Speech and Language Processing. HAL: https://inria.hal.science/hal-04567514/

Release Contributions: First version.

URL: https://github.com/Spruncкt/acoustic-sfw

Contact: Antoine Deleforge

6.1.2 opla

Name: One Page Layout Automator

Keywords: Python, Web

Functional Description: - Generate a professional webpage from a single markdown file - Handle publication lists coming from HAL database or from a bibtex file - Highly customizable thanks to the use of jinja templates, shortcodes and custom styles

Contact: Matthieu Boileau

6.1.3 LLG3D

Name: LLG3D

Keywords: 3D, Python, MPI, Micromagnetism, Landau-Lifshitz-Gilbert equation

Functional Description: LLG3D is a solver for the stochastic Landau-Lifshitz-Gilbert equation in 3D. It is written in Python and utilizes the MPI library to parallelize computations.

URL: https://llg3d.pages.math.unistra.fr/llg3d/

Contact: Matthieu Boileau

Partner: IPCMS

7 New results

7.1 Data driven solvers: Numerical methods for compressible flows

This section contains some works on numerical solvers which are currently not enhanced by ML technics but which are good candidate for that.

7.1.1 Implicit-explicit solver for a two-fluid single-temperature model

Participants: Andrea Thomann.

Reference: [14]

In this work, we have derived an analyzed a new implicit-explicit finite volume (RS-IMEX FV) scheme for a single-temperature SHTC model. We note that the two-fluid model allows two velocities and pressures. Further, it includes two dissipative mechanisms: phase pressure and velocity relaxations. In the proposed scheme these processes are treated differently. The relative velocity relaxation term is linear and is resolved as a part of the implicit sub-system, whereas the pressure relaxation is strongly nonlinear and therefore is treated separately by the Newton method. Our RS-IMEX FV method is constructed in such a way that acoustic-type waves are linearized around a suitably chosen reference state (RS) and approximated implicitly in time and by means of central finite differences in space. The remaining advective-type waves are approximated explicitly in time and by means of the Rusanov FV method. The RS-IMEX FV scheme is suitable for all Mach number flows, but in particular it is asymptotic preserving in the low Mach number flow regimes. Many multi-phase flows, such as granular or sediment transport flows, can be modeled within the single-temperature approximation. In turn, many of these flows are weakly compressible and therefore impose severe time step restrictions if solved with a time-explicit numerical scheme. Therefore, the proposed RS-IMEX FV scheme is suitable to model various environmental flows. The proposed method was tested on a number of test cases for low and moderately high Mach number flows demonstrating the capability of the scheme to properly capture both regimes. The theoretical second order accuracy of the scheme was confirmed on a stationary vortex test case. We compared the second order scheme against its first order variant which showed that the second order scheme yields more accurate approximations of discontinuities. Finally, the theoretically proven asymptotic preserving property was verified numerically.

7.1.2 A structure-preserving semi-implicit IMEX finite volume scheme for ideal magnetohydrodynamics at all Mach and Alfvén numbers

Participants: Andrea Thomann.

Reference: [5]

In this work, we present a divergence-free semi-implicit finite volume scheme for the simulation of the ideal magnetohydrodynamics (MHD) equations which is stable for large time steps controlled by the local transport speed at all Mach and Alfvén numbers. An operator splitting technique allows to treat the convective terms explicitly while the hydrodynamic pressure and the magnetic field contributions are integrated implicitly, yielding two decoupled linear implicit systems. The linearity of the implicit part is achieved by means of a semi-implicit time linearization. This structure is favorable as second-order accuracy in time can be achieved relying on the class of semi-implicit IMplicit–EXplicit Runge–Kutta (IMEX-RK) methods. In space, implicit cell-centered finite difference operators are designed to discretely preserve the divergence-free property of the magnetic field on three-dimensional Cartesian meshes. The new scheme is also particularly well suited for low Mach number flows and for the incompressible limit of the MHD equations, since no explicit numerical dissipation is added to the implicit contribution and the time step is scale independent. Likewise, highly magnetized flows can benefit from the implicit treatment of the magnetic fluxes, hence improving the computational efficiency of the novel method. The convective terms undergo a shock-capturing second order finite volume discretization to guarantee the effectiveness of the proposed method even for high Mach number flows. The new scheme is benchmarked against a series of test cases for the ideal MHD equations addressing different acoustic and Alfvén Mach number regimes where the performance and the stability of the new scheme is assessed.

7.1.3 Convergence of a hyperbolic thermodynamically compatible finite volume scheme for the Euler equations

Participants: Andrea Thomann.

Reference: [23]

We study the convergence of a novel family of thermodynamically compatible schemes for hyperbolic systems (HTC schemes) in the framework of dissipative weak solutions, applied to the Euler equations of compressible gas dynamics. Two key novelties of our method are i) entropy is treated as one of the main field quantities and ii) the total energy conservation is a consequence of compatible discretization and application of the Abgrall flux.

7.1.4 A fully well-balanced hydrodynamic reconstruction

Participants: Victor Michel-Dansac.

Reference: [4]

The present work focuses on the numerical approximation of the weak solutions of the shallow water model over a non-flat topography. In particular, we pay close attention to steady solutions with nonzero velocity. The goal of this work is to derive a scheme that exactly preserves these stationary solutions, as well as the commonly preserved lake at rest steady solution. These moving steady states are solution to a nonlinear equation. We emphasize that the method proposed here never requires solving this nonlinear equation; instead, a suitable linearization is derived. To address this issue, we propose an extension of the well-known hydrostatic reconstruction. By appropriately defining the reconstructed states at the interfaces, any numerical flux function, combined with a relevant source term discretization, produces a well-balanced scheme that preserves both moving and non-moving steady solutions. This eliminates the need to construct specific numerical fluxes. Additionally, we prove that the resulting scheme is consistent with the homogeneous system on flat topographies, and that it reduces to the hydrostatic reconstruction when the velocity vanishes. To increase the accuracy of the simulations, we propose a well-balanced high-order procedure, which still does not require solving any nonlinear equation. Several numerical experiments demonstrate the effectiveness of the numerical scheme.

7.1.5 Parallel kinetic schemes for conservation laws, with large time steps

Participants: Philippe Helluy, Victor Michel-Dansac.

Reference: [11]

We propose a new parallel Discontinuous Galerkin method for the approximation of hyperbolic systems of conservation laws. The method remains stable with large time steps, while keeping the complexity of an explicit scheme: it does not require the assembly and resolution of large linear systems for the time iterations. The approach is based on a kinetic representation of the system of conservation laws previously investigated by the authors. In this paper, the approach is extended with a subdomain strategy that improves the parallel scaling of the method on computers with distributed memory.

7.1.6 An entropy-stable and fully well-balanced scheme for the Euler equations with gravity

Participants: Victor Michel-Dansac, Andrea Thomann.

References: [19], [28]

[19] concerns the derivation of a numerical scheme to approximate weak solutions of the Euler equations with a gravitational source term. The designed scheme is proved to be fully well-balanced since it is able to exactly preserve all moving equilibrium solutions, as well as the corresponding steady solutions at rest obtained when the velocity vanishes. Moreover, the proposed scheme is entropy-preserving since it satisfies all fully discrete entropy inequalities. In addition, in order to satisfy the required admissibility of the approximate solutions, the positivity of both approximate density and pressure is established. Several numerical experiments attest the relevance of the developed numerical method.

In addition, in [28], we extended this work to general equations of states. When the system is equipped with a convex entropy and associated entropy inequality, it is also entropy-stable and positivity-preserving for all thermodynamic variables. An extension to high order accuracy is presented. Numerical test cases illustrate the performance of the new scheme, using six different equations of state as examples, four analytic and two tabulated ones.

7.1.7 A high-order, fully well-balanced, unconditionally positivity-preserving finite volume framework for flood simulations

Participants: Victor Michel-Dansac.

Reference: [20]

In this work, we present a high-order finite volume framework for the numerical simulation of shallow water flows. The method is designed to accurately capture complex dynamics inherent in shallow water systems, particularly suited for applications such as tsunami simulations. The arbitrarily high-order framework ensures precise representation of flow behaviors, crucial for simulating phenomena characterized by rapid changes and fine-scale features. Thanks to an ad-hoc reformulation in terms of production-destruction terms, the time integration ensures positivity preservation without any time-step restrictions, a vital attribute for physical consistency, especially in scenarios where negative water depth reconstructions could lead to unrealistic results. In order to introduce the preservation of general steady equilibria dictated by the underlying balance law, the highorder reconstruction and numerical flux are blended in a convex fashion with a well-balanced approximation, which is able to provide exact preservation of both static and moving equilibria. Through numerical experiments, we demonstrate the effectiveness and robustness of the proposed approach in capturing the intricate dynamics of shallow water flows, while preserving key physical properties essential for flood simulations.

7.1.8 Composite unstructured meshes with source term

Participants: Emmanuel Franck.

Reference: [6]

In this work we focus on an adaptation of the composite method in order to deal with source term in the 2D Euler equations. This method extends classical 1D solvers (such as VFFC, Roe, Rusanov) to the two-dimensional case on unstructured meshes. The resulting schemes are said to be composite as they can be written as a convex combination of a purely node-based scheme and a purely edge-based scheme. We combine this extension with the ideas developed by Alouges, Ghidaglia and we propose two attempts at discretizing the source term of the Euler equations in order to better preserve stationary solutions. We compare these discretizations with the “usual” centered discretization on several numerical examples.

7.1.9 Maximum principle for the mass fraction in a system with two mass balance equations

Participants: Philippe Helluy.

Reference: [13]

In this paper written with EDF colleagues, we show how to improve the robustness of the computation of the mass fraction in the thermohydraulic EDF THYC software.

7.2 Lattice Boltzmann solvers

7.2.1 Reducing the memory usage of lattice-Boltzmann schemes with a DWT-based compression

Participants: Clément Flint, Philippe Helluy.

References: [8, 9]

We develop a new on-the-fly compression strategy for accelerating CFD computations. The resulting scheme is optimized for GPU computations. In a standard lattice-Boltzmann simulation, it allows reducing the memory footprint by an order of magnitude with a moderate impact on the computation time.

7.2.2 Stability analysis of the vectorial lattice-Boltzmann method (LBM)

Participants: Philippe Helluy.

References: [12]

We provide a fully rigorous entropy stability analysis of the vectorial Lattice-Boltzmann method. We also develop a new equivalent equation approach for studying the high-order consistency of the method.

7.2.3 Fourth-order entropy-stable lattice Boltzmann schemes for hyperbolic systems

Participants: Thomas Bellotti, Philippe Helluy, Laurent Navoret.

References: [18]

We construct a fourth-order entropy stable LBM scheme and apply it to compressible flows.

7.3 Data driven solvers: Hybrid solvers between classical approaches and machine learning

This section contains some works on the hybridation between classical numerical solvers and ML methods.

7.3.1 Accelerating the convergence of Newton's method for nonlinear elliptic PDEs using Fourier neural operators

Participants: Joubine Aghili, Victor Michel-Dansac, Vincent Vigon, Emmanuel Franck.

Reference: [2]

It is well known that Newton's method can struggle to converge if the initial guess is too far from the solution. Such a problem occurs in particular when this method is used to solve nonlinear elliptic PDEs discretized by finite differences. This work focuses on accelerating the convergence of Newton's method in this context. We use Fourier Neural Operator (FNO) to construct an approximation of the discrete solution of a PDE from its parameters. This approximation is then used as an initial guess for Newton's method. Numerical results, in one and two dimensions, show that the proposed initial guess accelerates the convergence of Newton's method by a significant margin compared to a naive initial guess, especially for highly nonlinear and anisotropic problems, with larger gains on coarse grids.

7.3.2 Approximately well-balanced discontinuous Galerkin methods using bases enriched with physics-informed neural networks

Participants: Emmanuel Franck, Victor Michel-Dansac, Laurent Navoret.

Reference: [10]

This work concerns the enrichment of Discontinuous Galerkin (DG) bases, so that the resulting scheme provides a much better approximation of steady solutions to hyperbolic systems of balance laws. The basis enrichment leverages a prior – an approximation of the steady solution – which we propose to compute using a Physics-Informed Neural Network (PINN). To that end, after presenting the classical DG scheme, we show how to enrich its basis with a prior. Convergence results and error estimates follow, in which we prove that the basis with prior does not change the order of convergence, and that the error constant is improved. To construct the prior, we elect to use parametric PINNs, which we introduce, as well as the algorithms to construct a prior from PINNs. We finally perform several validation experiments on four different hyperbolic balance laws to highlight the properties of the scheme. Namely, we show that the DG scheme with prior is much more accurate on steady solutions than the DG scheme without prior, while retaining the same approximation quality on unsteady solutions.

7.4 Data driven solvers: Neural network based methods for PDE

This subsection contains some works on pure ML solvers for PDE which is also a sub axis of the data driven solver axis.

7.4.1 A dynamical neural Galerkin scheme for filtering problems

Participants: Joubine Aghili.

References: [17]

This work explores reconstructing the state of a dynamic system from partial observations, using a model based on a physical PDE with unknown parameters. We introduce a filtering method where a neural network, whose parameters are updated with observational data, approximates the dynamics. This not only estimates the system's state but also tracks changes in PDE parameters over time. We demonstrate this with a one-dimensional Korteweg-de Vries (KdV) equation, highlighting how the placement and number of sensors significantly impact results, suggesting the need for dynamic sensor positioning.

7.4.2 Volume-preserving geometric shape optimization of the Dirichlet energy using variational neural networks

Participants: Victor Michel-Dansac, Emmanuel Franck.

Reference: [3]

In this work, we explore the numerical solution of geometric shape optimization problems using neural network-based approaches. This involves minimizing a numerical criterion that includes solving a partial differential equation with respect to a domain, often under geometric constraints like a constant volume. We successfully develop a proof of concept using a flexible and parallelizable methodology to tackle these problems. We focus on a prototypical problem: minimizing the so-called Dirichlet energy with respect to the domain under a volume constraint, involving Poisson's equation in $\mathbb{R}^2$. We use variational neural networks to approximate the solution to Poisson's equation on a given domain, and represent the shape through a neural network that approximates a volume-preserving transformation from an initial shape to an optimal one. These processes are combined in a single optimization algorithm that minimizes the Dirichlet energy. A significant advantage of this approach is its inherent parallelizability, which makes it easy to handle the addition of parameters. Additionally, it does not rely on shape derivative or adjoint calculations. Our approach is tested on Dirichlet and Robin boundary conditions, parametric right-hand sides, and extended to Bernoulli-type free boundary problems. The source code for solving the shape optimization problem is open-source and freely available here.

7.5 Data-driven optimal control and inverse problems: Ferromagnetic modelisation

This section contains wome work on PDE problem with control objective. For now the ML part is not began.

7.5.1 Micromagnetic simulations of the size dependence of the Curie temperature in ferromagnetic nanowires and nanolayers

Participants: Clémentine Courtès, Mathieu Boileau.

Reference: [7]

We solved the Landau-Lifshitz-Gilbert equation in the finite-temperature regime, where thermal fluctuations are modeled by a random magnetic field whose variance is proportional to the temperature. We obtained Curie temperatures that are in line with the experimental values for cobalt, iron and nickel and for finite-sized objects such as nanowires (1D) and nanolayers (2D), we study the variances of the Curie temperature with respect to the smallest size of the system. Moreover, optimization and parallelization of the python code solving the Landau-Lifshitz-Gilbert equation in the finite-temperature regime led to a 100-time acceleration of the code. We were therefore able to study the effect of the size of the material on the magnetization, in particular the value of the Curie temperature.

7.5.2 Existence and uniqueness of domain walls for notched ferromagnetic nanowires

Participants: Clémentine Courtès.

Reference: [22]

In this work we investigate a simple model of notched ferromagnetic nanowires using tools from calculus of variations and critical point theory. Specifically, we focus on the case of a single unimodal notch and establish the existence and uniqueness of the critical point of the energy. This is achieved through a lifting argument, which reduces the problem to a generalized Sturm-Liouville equation. Uniqueness is demonstrated via a Mountain-Pass argument, where the assumption of two distinct critical points leads to a contradiction. Additionally, we show that the solution corresponds to a system of magnetic spins characterized by a single domain wall localized in the vicinity of the notch. We further analyze the asymptotic decay of the solution at infinity and explore the symmetric case using rearrangement techniques.

7.6 Data driven modeling: Data-driven reduced modeling and PDE discovery

This subsection contains some works on reduced modeling and model discovery using ML.

7.6.1 Generalizing the SINDy approach with nested neural networks

Participants: Clément Flint, Emmanuel Franck, Victor Michel-Dansac.

Reference: [25]

Symbolic Regression (SR) is a widely studied field of research that aims to infer symbolic expressions from data. A popular approach for SR is the Sparse Identification of Nonlinear Dynamical Systems (SINDy) framework, which uses sparse regression to identify governing equations from data. This study introduces an enhanced method, Nested SINDy, that aims to increase the expressivity of the SINDy approach thanks to a nested structure. Indeed, traditional symbolic regression and system identification methods often fail with complex systems that cannot be easily described analytically. Nested SINDy builds on the SINDy framework by introducing additional layers before and after the core SINDy layer. This allows the method to identify symbolic representations for a wider range of systems, including those with compositions and products of functions. We demonstrate the ability of the Nested SINDy approach to accurately find symbolic expressions for simple systems, such as basic trigonometric functions, and sparse (false but accurate) analytical representations for more complex systems. Our results highlight Nested SINDy's potential as a tool for symbolic regression, surpassing the traditional SINDy approach in terms of expressivity. However, we also note the challenges in the optimization process for Nested SINDy and suggest future research directions, including the designing of a more robust methodology for the optimization process. This study proves that Nested SINDy can effectively discover symbolic representations of dynamical systems from data, offering new opportunities for understanding complex systems through data-driven methods.

7.7 Data-driven optimal control and inverse problems: Inverse problems

7.7.1 Fully reversing the shoebox image source method: from impulse responses to room parameters

Participants: Antoine Deleforge, Tom Sprunck.

Reference: [30]

We developped an algorithm that fully reverses the shoebox image source method (ISM), a popular and widely used room impulse response (RIR) simulator for cuboid rooms introduced by Allen and Berkley in 1979. More precisely, given a discrete multichannel RIR generated by the shoebox ISM for a microphone array of known geometry, the algorithm reliably recovers the 18 input parameters. These are the 3D source position, the 3 dimensions of the room, the 6-degrees-of-freedom room translation and orientation, and an absorption coefficient for each of the 6 room boundaries. The approach builds on a recently proposed gridless image source localization technique combined with new procedures for room axes recovery and first-order-reflection identification. Extensive simulated experiments reveal that near-exact recovery of all parameters is achieved for a 32-element, 8.4-cm-wide spherical microphone array and a sampling rate of 16 kHz using fully randomized input parameters within rooms of size 2x2x2 to 10x10x5 meters. Estimation errors decay towards zero when increasing the array size and sampling rate. The method is also shown to strongly outperform a known baseline, and its ability to extrapolate RIRs at new positions is demonstrated. Crucially, the approach is strictly limited to low-passed discrete RIRs simulated using the vanilla shoebox ISM. Nonetheless, it represents to our knowledge the first algorithmic demonstration that this difficult inverse problem is in principle fully solvable over a wide range of configurations.

7.8 Others

7.8.1 Phi-FD : A well-conditioned finite difference method inspired by Phi-FEM for general geometries on elliptic PDEs

Participants: Vincent Vigon.

References: [24]

This work presents a new finite difference method, called Phi-FD, inspired by the Phi-FEM approach for solving elliptic PDEs on general geometries. The proposed method uses Cartesian grids, ensuring simplicity in implementation. Moreover, contrary to the previous finite difference scheme on non-rectangular domains, the associated matrix is well-conditioned. The use of a level-set function for the geometry description makes this approach relatively flexible. We prove the quasi-optimal convergence rates in several norms and the fact that the matrix is well-conditioned. Additionally, the paper explores the use of multigrid techniques to further accelerate the computation. Finally, numerical experiments in both 2D and 3D validate the performance of the Phi-FD method compared to standard finite element methods and the Shortley-Weller approach.

7.8.2 Latent watermarking of audio generative models

Participants: Antoine Deleforge.

Reference: [29]

The advancements in audio generative models have opened up new challenges in their responsible disclosure and the detection of their misuse. In response, we introduced a method to watermark latent generative models by a specific watermarking of their training data. The resulting watermarked models produce latent representations whose decoded outputs are detected with high confidence, regardless of the decoding method used. This approach enables the detection of the generated content without the need for a post-hoc watermarking step. It provides a more secure solution for open-sourced models and facilitates the identification of derivative works that fine-tune or use these models without adhering to their license terms. Our results indicate for instance that generated outputs are detected with an accuracy of more than 75% at a false positive rate of less than 0.1%, even after fine-tuning the latent generative model.

8 Bilateral contracts and grants with industry

8.1 Bilateral Grants with Industry

Participants: Philippe Helluy.

We collaborate with EDF through the CIFRE thesis of Gauthier Lazare in the optimization of nuclear plant simulation software. The optimization is realized through algorithmic improvements but also with software acceleration based on machine learning.

9 Partnerships and cooperations

9.1 International initiatives

9.1.1 Inria associate team not involved in an IIL or an international program

Participants: Clémentine Courtès.

Inria associate team PANDA (2024-2026). Coordinator: A. de Laire (Université de Lille). MACARON participant: Clémentine Courtès. Study of dispersive PDE systems for wave propagation.

9.2 International research visitors

9.2.1 Visits to international teams

Research stays abroad

Andrea Thomann

Visited institution: University of Verona

Country: Italy

Dates: November 2024

Context of the visit: Collaboration

Mobility program/type of mobility: Research stay

9.3 European initiatives

9.3.1 Other european programs/initiatives

ANR-DFG MILK (Machine Learning for Kinetic equations)

Participants: Clémentine Courtès, Emmanuel Franck, Laurent Navoret.

Dates: 01/2022 – 12/2024.
Coordinators: Emmanuel Franck and E. Sonnendrücker (Technische Universität München).
Partners: MACARON and Technische Universität München
Decription: Kinetic models are accurate descriptions of interacting particle systems in physics. However, their numerical resolution is often too demanding, as they are defined in the large-dimensional

position/velocity phase space and involve multi-scale dynamics. For this reason, reduced models have been developed that represent optimal trade-offs between numerical cost and modeling completeness. In general, this reduction is carried out in two ways. The first is based on asymptotic models that filter out fast dynamics and are obtained when a small parameter tends towards zero (collision/oscillation limit). The second, called reduced order modeling, consists in finding a smaller representation of the problem able to describe the dynamics (POD). The main objective of this project is to design new reduced order models that are more efficient than classical ones, based on machine learning techniques applied to kinetic data. Ensuring the stability of the obtained models will be a key point of these studies.

9.4 National initiatives

9.4.1 ANR MOSICOF (MOdeling and SImulation of COmplex Ferromagnetic systems)

Participants: Clémentine Courtès.

Dates: 10/2021 – 10/2025.
Coordinator: S. Labbé, Sorbonne Université.
Partners: Sorbonne université, Université de Pau et des Pays de l'Adour, Université de Strasbourg
Decription: During the last decade, promising applications of ferromagnetic materials have emerged in the domains of nanoelectronics (spintronic) and data storage: complex ferromagnetic systems are increasingly used for digital data recording and logic devices. They reduce the energy storage cost while improving the performance of the devices. The goal of this proposal is to bring together mathematicians and physicists around the understanding of the properties of ferromagnetism. One of the main objectives is to highlight and treat new multi-physics models, allowing for optimization and control of the magnetizations, and to simulate the phenomena in a more efficient and less expensive way. We wish to develop approaches leading to mathematically justified and physically relevant solutions for the analysis and optimization of these materials, and which could ultimately lead to implementation on devices.

9.4.2 ANR JCJC SMEAGOL (Méthode structurelle – Application à des systèmes hyperboliques généraux)

Participants: Victor Michel-Dansac.

Dates: 11/2024 – 10/2028.
Funding: 283 k€
Coordinator: Victor Michel-Dansac
Decription: The structural method, introduced over the last two years, develops high-order numerical schemes for solving PDEs on compact stencils. This finite difference approach is unique in that it approximates both the solution and its derivatives with the same order of accuracy by defining two independent sets of discrete equations: the physical equations (PEs) and the structural equations (SEs). The PEs represent the problem's physics, while SEs ensure the accuracy of the discretization. This separation provides a high degree of flexibility, allowing for the modification of PEs to include specific constraints (e.g., ensuring a vector field is divergence-free) and the adjustment of SEs to handle non-smooth solutions or enhance stability. The ANR project SMEAGOL seeks to extend this method to hyperbolic systems of balance laws in multiple spatial dimensions, where continuous initial conditions often lead to non-smooth solutions and multiscale regime changes. This makes the method particularly suitable for complex problems in fluid mechanics or electromagnetism. The separation between physical and structural equations in this framework allows for the dynamic adaptation of the scheme to the local problem, switching PEs or SEs on or off as needed. SMEAGOL's goals include both constructing and adapting the structural method to these advanced applications, to develop well-balanced, asymptotic-preserving and robust schemes.

9.4.3 ANR MAPEFLU (Modelling the effect of Apoptosis on Epithelium FLUidity)

Participants: Laurent Navoret.

Dates: 03/2023–02/2027
Coordinator: Laurent Navoret
Partners: Institut Pasteur, Université Paris Université de Strasbourg (IRMA, IGBMC)
Decription: Epithelia have a viscoelastic behaviour: they respond as solids over short times and as fluids over large times. This fluidity plays an essential role in morphogenesis and tissue deformation. At the cellular scale, fluidity is achieved by the remodelling of junctions between cells due to their interactions but also by cell division and death. However, the contribution of apoptosis to fluidity has been little studied and remains unclear since cell death is also associated with local elastic constraints. Our project first aims at developing a novel particle model, describing cell cycles and the polarities interactions (Vicsek-like model), to assess the impact of cell death rate on tissue fluidity. The construction of this model will be strongly guided by comparisons with in vitro (MDCK cells) and in vivo (Drosophila pupa) experiments. From this particle model, a hydrodynamic model will be rigorously derived and simulations based on this new macroscopic description will be utilized to improve the understanding of tissue dynamics. The present study will thus provide a generic model, consistent with the experimental data and allowing one of the first systematic assessments of the role of apoptosis in tissues.

9.4.4 ANR SIMBADNESTICOST (Simulation Based Network Structure Inference Constrained by Observed Spike Trains)

Participants: Vincent Vigon.

Dates: 2023 - 2026
Grant: 159 k€
Coordinator: Christophe Pouzat
Partners: IRMA (Institut de recherche en mathématique avancées) and University of Strasbourg
Decription: Neurophysiologists are now able to record from a large number of electrodes the sequences of action potentials generated by many neurons. Unfortunately, these "many neurons" still represent only a tiny fraction of the neuronal population that constitutes the network. By using association statistics such as the estimation of cross-correlation functions, they attempt to infer the structure of the network formed by the recorded neurons. This produces a "network image" generally called a "functional network" whose characteristics strongly depend on the recording conditions. We consider that reconstructing the network formed by the recorded neurons is an ill-posed problem. We propose to focus instead on the "generative probability distribution" of the network: what is the probability of having a connection from a type A neuron to a type B neuron?

9.4.5 ANR PHI-FEM (Développement d'une méthode aux éléments finis pour la conception de jumeaux numériques temps réel en chirurgie)

Participants: Vincent Vigon.

Dates: 2023 - 2026
Grant: 324 k€
Coordinator: Michel Duprez
Partners: Inria teams MACARON and MIMESIS.
Decription: Phi-FEM is a recently proposed finite element method for the efficient numerical solution of partial differential equations in domains defined by level-set functions. The main objective of this

project is to develop Phi-FEM into an efficient, patient-specific, and real-time simulation tool for human organs. To achieve this goal, we will adapt Phi-FEM to equations relevant to biomechanics, provide an efficient implementation allowing the use of real organ geometries, and finally combine it with convolutional neural networks to make it real-time after training.

9.4.6 ANR HAIKUS (Artificial Intelligence applied to augmented acoustic Scenes)

Participants: Antoine Deleforge.

Dates: 12/2019 - 12/2024
Coordinator: Olivier Warsufel (Ircam, Paris)
Partners: Ircam (Paris), Inria (Nancy), IJLRA (Paris)
Decription: HAIKUS aims to achieve seamless integration of computer-generated immersive audio content into augmented reality (AR) systems. One of the main challenges is the rendering of virtual auditory objects in the presence of source movements, listener movements and/or changing acoustic conditions.

9.4.7 ANR JCJC DENISE (Tackling hard problems in audio using Data-Efficient Non-linear InverSe mEthods)

Participants: Antoine Deleforge.

Dates: 10/2020 – 12/2024
Coordinator: Antoine Deleforge
Decription: DENISE aims to explore the applicability of recent breakthroughs in the field of nonlinear inverse problems to audio signal reparation and to room acoustics, and to combine them with compact machine learning models to yield data-efficient techniques.

9.4.8 PEPR IA/PC IA-EDP

Participants: Philippe Helluy, Joubine Aghili, Clémentine Courtès, Emmanuel Franck, Victor Michel-Dansac, Vincent Vigon, Laurent Navoret.

Dates: 01/09/2023 – 31/08/2027
Coordinator: A. Chambolle (Univ. Paris-Dauphine)
Decription: The PEPR IA is a large national project on artificial intelligence (AI). The PC IA-PDE is a project funded by the ANR, which gathers ten major French institutions involved in developing the mathematical analysis of AI, the study of optimization in machine learning, as well as in developing machine learning for numerical analysis and scientific computing. We will study the link between modern AI methods and optimal control, optimal transport, PDE and numerical analysis. The team is involved in the optimal control aspect.

9.4.9 PEPR Numpex/PC Exa-MA

Participants: Philippe Helluy, Joubine Aghili, Clémentine Courtès, Emmanuel Franck, Victor Michel-Dansac, Vincent Vigon, Laurent Navoret.

Dates: 10/2021 – 10/2025.
Coordinator: Christophe Prud'homme
Decription: The Exa-MA project focuses on the Exascale aspects of digital methods, guaranteeing their adaptability to existing and future hardware. It is also a cross-disciplinary project, proposing methods and tools in which modelling, data and AI, through algorithms, are central. The team is mainly involved in the WP2 on reduced modeling and ML technics but also in the WP1 on numerical methods

9.5 Regional initiatives

Participants: Joubine Aghili.

Dates: 02/2024 – 02/2025.
Grant: 55 k€
Coordinator: Joubine Aghili
Partners: MACARON (Inria) and iCube (University of Strasbourg)
Decription: Recruitment of a Research Engineer to develop a direct and inverse problem code in Python to simulate radiative transfert in a turbid media.

10 Dissemination

Participants: Philippe Helluy, Antoine Deleforge, Joubine Aghili, Clémentine Courtès, Emmanuel Franck, Victor Michel-Dansac, Vincent Vigon, Andrea Thomann, Laurent Navoret.

10.1 Promoting scientific activities

10.1.1 Scientific events: organisation

- Member of organizing commitee of PANDA-Hyp workshop, Arcachon, France, oct. 2024 (A. Thomann). More information.
- Co-organization of the 21st International Congress on Mathematical Physics (ICMP) : July 2024, Palais des Congrès, Strasbourg (C. Courtès). More information.
- Co-organization of two mini-symposia "Models and asymptotics for ferromagnetic materials" : May 2024, CANUM2024, Ile de Ré (C. Courtès). More information.
- Organization of the workshop on Scientific Machine Learning, Strasbourg, approx. 60 participants, June 2024 (V. Michel-Dansac, L. Navoret, E. Franck). More information.
- Organization of the summer school « New trends in computing » (L. Navoret). More information.
- Co-organization of the 6th workshop IRMA-EDF on compressible multiphase flows, June 2024 (P. Helluy). More information.
- Co-organization of the workshop "Methodological advances for Audio Augmented Reality and its applications" at IRCAM, Paris, France, approx. 40 participants, December 2024 (A. Deleforge). More information.
- Co-organization of the regular ITI IRMIA++ seminars since Sept. 2024, Strasbourg university (C. Courtès, L. Navoret).
- Co-organization of the regular sem'in (internal seminar of the laboratory) since Sept. 2023, Strasbourg university (C. Courtès).

- Organization of the weekly MACARON/MOCO seminar since Sept. 2021 (C. Courtès, V. Michel-Dansac, J. Aghili).

10.1.2 Scientific events: selection

Member of the conference program committees

- Meta-reviewer and area chair for the International Conference on Acoustics, Speech and Signal Processing (ICASSP) (A. Deleforge)

Reviewer

- Reviewer for the summer school « CEMRACS2024 » (J. Aghili)
- Reviewer for the International Conference on Acoustics, Speech and Signal Processing (ICASSP) (A. Deleforge)

10.1.3 Journal

Member of the editorial boards

- Associate Editor for the EURASIP Journal on Audio, Speech, and Music Processing (A. Deleforge)
- Editor for ESAIM proceedings, CEMRACS 2022 - Transport in physics, biology and urban traffic, volume 77. (E. Franck, L. Navoret)

Reviewer - reviewing activities

- ESAIM:M2AN (A. Thomann, C. Courtès)
- Journal of Computational Physics (A. Thomann, L. Navoret, P. Helluy, E. Franck)
- Journal of Scientific Computing (A. Thomann)
- Mathematical Methods in the Applied Sciences (A. Thomann)
- SIAM Journal on Scientific Computing (A. Thomann)
- Applied Mathematics and Computation (C. Courtès)
- Mathematical Reviews/MathScinet (C. Courtès, V. Michel-Dansac)
- Mathematics and Computers in Simulation (V. Michel-Dansac)
- SMAI Journal on Computational Mathematics (V. Michel-Dansac, E. Franck)
- zbMath (V. Michel-Dansac)
- ESAIM Proceedings (L. Navoret, P. Helluy, E. Franck)
- CALCOLO (J. Aghili, E. franck)
- Journal of Engineering Mathematics (J. Aghili)
- AIAA Journal (P. Helluy)
- IEEE Transactions on Acoustics Speech and Signal Processing (A. Deleforge)
- Applied Acoustics (A. Deleforge)
- Robotics and Autonomous Systems (A. Deleforge)

10.1.4 Invited talks

International Audience

- Plenary talk at the international workshop "PANDA Lille-Santiago", September, Universidad de Chile, Santiago, Chile, (online) (C. Courtès)
- Plenary Talk at the international seminar "SPP-2410 Young Scientists Retreat", September, Hirschegg, Austria (V. Michel-Dansac)
- Plenary Talk at the thematic days "MIRES", March, Poitiers, France (V. Michel-Dansac)
- Talk at the international conference "ALGORITMY 2024", March, Slovakia (V. Michel-Dansac)
- Plenary talk at the international workshop "Deep Learning in Inverse Problems", September, Hambourg, Germany (A. Deleforge)
- Plenary talk at the international workshop "Methodological advances for Audio Augmented Reality and its applications", December, IRCAM, Paris, France (A. Deleforge)
- Plenary Talk at the Conference "Numerical Methods for the kinetic equations of Plasma Physics (Numkin)"", November, Garching, Germany (L. Navoret)
- Talk at the international workshop: "the conference "New trends in the numerical analysis of PDEs", June 2024, Lille, France. (E. Franck)
- Plenary talk at the workshop: "Boundaries, Multiscale dynamics, and Stochastic (BMS)", May, Rennes, France (P. Helluy)

National Audience

- Plenary talk at the conference "New Trends in the Numerical Analysis of Partial Differential Equations", Lille, France (A. Thomann)
- Plenary talk at the workshop "Oberwolfach Workshop 2409 - Hyperbolic Balance Laws: Interplay between Scales and Randomness", Oberwolfach, Germany (A. Thomann)
- Plenary talk at the conference "ProHyp 2024, 3rd international workshop on Perspectives on multiphase fluid dynamics, continuum mechanics and hyperbolic balance laws", Trento, Italy (A. Thomann)
- Plenary talk at the Workshop "INdAM workshop Innovations in Numerics for Stiff DEs", Rome, Italy (A. Thomann)
- Plenary talk at the workshop "Modeling, theory and numerics for PDEs (kinetic and hyperbolic systems)", October, Aussois, France (C. Courtès)
- Talk at the annual workshop of the ANR MOSICOF project, June, Sorbonne Université, Paris, France (C. Courtès)
- Plenary Talk at the workshop "MEDIA", December, Toulon, France (V. Michel-Dansac)
- Plenary Talk at the workshop "École RT T&E", November, Nouan-le-Fuzelier, France (V. Michel-Dansac)
- Plenary Talk at Journée "EMS : EDP, modélisation, simulation", September, Orléans, France (L. Navoret)
- Plenary Talk at Workshop "Modeling, theory and numerics for PDEs", October, Aussois, France (L. Navoret)
- Talk at the workshop: "Journée "fondement de l'IA: PINNs", January, Paris, France.(E. Franck)

- Talk at the workshop: "Journée thématiques MIRES, Réseaux de neurones et applications", March, Poitiers, France.(E. Franck)
- Talk at the workshop: "En l'honneur de François Dubois", October, Paris, France. (E. Franck)
- Talk at the workshop: "Journée PEPR IA-NUMPEX-DIADEM", November, Paris, France. (E. Franck)

Seminar talks

- Talk at the seminar "Numerical methods for plasma physics seminar", Max Planck Institute for Plasma Physics, Garching, Munich, Germany (A. Thomann)
- Talk at the seminar "ATLANTIS", February, Sophia-Antipolis, France (V. Michel-Dansac)
- Talk at the seminar "MOD", May, Limoges, France (V. Michel-Dansac)
- Talk at the seminar "Calcul Scientifique et Modélisation", May, Bordeaux, France (V. Michel-Dansac)
- Talk at the seminar "Rencontres INRIA-LJLL en calcul scientifique", May, LJLL, Paris, France (C. Courtès)
- Talk at the internal seminar of IRMA, April, IRMA, Université de Strasbourg, France (C. Courtès)
- Talk at the seminar of "Non-linear analysis and optimisation", April, LMA, Université d'Avignon, France (C. Courtès)
- Talk at the seminar of "Numerical analysis and PDE", February, Laboratoire Paul Painlevé, Université de Lille, France (C. Courtès)
- Talk at the seminar "POEMS", February, INRIA, ENSTA, Paris, France (C. Courtès)
- Talk at the seminar "Infomath", April, LPSM, Paris, France (M. Boileau)
- Talk at the Seminar "EDP", November, Metz, France (L. Navoret)
- Talk at the Seminar: "ENSTA EDP", Saclay, October, France. (E. Franck)
- Talk at the Seminar: "numerical analysis CNAM", October, Paris, France. (E. Franck)
- Talk at the Seminar: "LBM", May, Paris, France. (E. Franck)
- Talk at the Seminar: "numerical analysis Waterloo", October, Paris, France. (E. Franck)
- 3 Lectures at the "mathematical fluid mecanics" seminar of the university of Würzburg, February, Germany (P. Helluy)

10.1.5 Leadership within the scientific community

- Leader of the Research Group (GdR) "Calcul" (M. Boileau)

10.1.6 Scientific expertise

- One project review for the Swiss scientific foundation (P. Helluy)

10.1.7 Research administration

- Nominated member of the IRMA Laboratory Council, Strasbourg university (C. Courtès)
- Elected member of the Mathematicians Commission of the university of Strasbourg (C. Courtès, L. Navoret)
- Nominated member at the Inria Nancy - Grand Est center committee (C. Courtès)
- Referent, co-responsible and member on laboratory parity for INSMI, the mathematics and computer science faculty (UFR math-info) and IRMA (C. Courtès)
- Responsible of training for Institut Thématique Interdisciplinaire IRMIA++, Strasbourg university (L. Navoret)
- Elected member of the expert committee, UFR Math-Info, Université de Strasbourg (L. Navoret, J. Aghili)
- Head of the IRMA MOCO team (P. Helluy)
- Referent on research data for the Inria Nancy - Grand Est center (A. Deleforge)
- Board member of the Research Group (GdR) "Calcul" (E. Franck)
- Member of the COMIPERS, Inria Nancy - Grand Est (E. Franck)

10.2 Teaching - Supervision - Juries

10.2.1 Teaching

- 28h Methodes numeriques pour les EDP 2, Master 2 on Scientific Computing (M2 CSMI) at UFR Maths-Info, Strasbourg university (A. Thomann)
- 8h TP Numerical resolution techniques for engineering, M1 CSMI at UFR Maths-Info, Strasbourg university (A. Thomann)
- 37h of CM on computer science in L3 magistère at UFR Maths-Info, Strasbourg university (C. Courtès)
- 28h of TD on computer science in L3 magistère at UFR Maths-Info, Strasbourg university (C. Courtès)
- 15h of CM on numerical analysis in L3 mathématiques at UFR Maths-Info, Strasbourg university (C. Courtès)
- 36h of TD on numerical analysis in L3 mathématiques at UFR Maths-Info, Strasbourg university (C. Courtès)
- 8h of TD on real analysis in L2 informatique at UFR Maths-Info, Strasbourg university (C. Courtès)
- 8h of TP on real analysis in L2 informatique at UFR Maths-Info, Strasbourg university (C. Courtès)
- Responsible of the option "mathématiques et statistiques pour préparer aux concours administratifs" of L3, UFR Maths-Info and Institut de Préparation à l'Administration Générale, Strasbourg (C. Courtès)
- 6h of "textes" in M2 Agrégation at UFR Maths-Info, Strasbourg university (V. Michel-Dansac)
- 14h of CM in Intro to Object-Oriented Programming in L2 informatique at UFR Maths-Info, Strasbourg university (V. Michel-Dansac)
- 14h of TP in Scientific Computing in M1 CSMI at UFR Maths-Info, Strasbourg university (V. Michel-Dansac)

- 36h of TD, C++ L3 informatique at UFR Maths-Info, Strasbourg university (E. Franck)
- 28 of CI, SciML2 M2 CSMI at UFR Maths-Info, Strasbourg university (E. Franck)
- 16h of CM in “Basics in mathematics” in M2 Cell Physics at Strasbourg university (L. Navoret)
- 4h of CM in “Math for living matter” in M2 Cell Physics at Strasbourg university (L. Navoret)
- 12h of CM in “Scientific computing” in Master 2 Agrégation at Strasbourg university (L. Navoret)
- 9h of TD in “Scientific computing” in Master 2 Agrégation at Strasbourg university (L. Navoret)
- 28h of CI in "Scientific computing (sparse linear algebra)" in Master 2 Scientific Computing (M2 CSMI) at Strasbourg university (L. Navoret)
- 6h of TD in "Interdisciplinary seminars" in Diplôme d’université at Strasbourg university (L. Navoret)
- 4h of TD in « Interdisciplinary project » in Diplôme d’université at Strasbourg university (L. Navoret)
- 56h of CI in Mathematics for sciences II in L1 at UFR Maths-Info, Strasbourg university (J. Aghili)
- 7h of CI in Projet management in M1 CSMI at UFR Maths-Info, Strasbourg university (J. Aghili)
- 63h of CI in Numerical Analysis and Computer sciences at UFR Physics and Engineering, Strasbourg university (J. Aghili)
- 10h of TD in Numerical Analysis in Prépa Agregation of Mathematics at UFR Maths-Info, Strasbourg university (J. Aghili)
- 63h of CI in Mathematics for sciences I in L1 at UFR Maths-Info, Strasbourg university (J. Aghili)
- 7h of CI in Projet management in M2 CSMI at UFR Maths-Info, Strasbourg university (J. Aghili)
- 8h of TP in Numerical Methods in M1 CSMI at UFR Physics and Engineering, Strasbourg university (J. Aghili)
- 6h of course in the Summer school « New trends in computing », ITI IRMIA++, Strasbourg university (M. Boileau)
- 18h of Python for Data Science, M2 CSMI at UFR Math-Info, Strasbourg university (M. Boileau)
- 60h of CI. Modelisation Probabiliste en M2 Agreg, UFR Maths-Info, Strasbourg university (V. Vigon)
- 35h of CI. Traitement et exploitation des données. M1 CSMI, UFR Maths-Info, Strasbourg university (V. Vigon)
- 35h of CI. Traitement du signal et des images 1. M1 CSMI, UFR Maths-Info, Strasbourg university (V. Vigon)
- 35h of CI. Traitement du signal et des images 2. M2 CSMI, UFR Maths-Info, Strasbourg university (V. Vigon)
- 35h of CI. Science des données pour l’actuariat, M2 Actuariat, UFR Maths-Info, Strasbourg university (V. Vigon)
- 16h of TP on computer assisted proof in M1 CSMI at UFR Math-Info, Strasbourg university (P. Helluy)
- 20h of CM in C++ in L3 informatique, UFR Math-Info, Strasbourg university (P. Helluy)
- 28h of CI in scientific computing in M1 CSMI, UFR Math-Info, Strasbourg university (P. Helluy)

- 10,5h of CM on Artificial Intelligence, Machine Learning, Deep Learning in M1 at Telecom-Physique Strasbourg (A. Deleforge)
- 12h of TP on Artificial Intelligence, Machine Learning, Deep Learning in M1 at Telecom-Physique Strasbourg (A. Deleforge)
- 12h of TP on Artificial Intelligence, Machine Learning, Deep Learning in M1 at Telecom-Physique Strasbourg (A. Deleforge)
- 12h of TP on Unsupervized Machine Learning in L3 at Telecom-Physique Strasbourg (A. Deleforge)
- 7h of CM on Artificial Intelligence and Statistical Learning in M1 at Telecom-Physique Strasbourg (A. Deleforge)

10.2.2 Supervision

- PostDoc Dinh Hung Truong, 2023-, "Design of Neural Operators based on PINNs; applications to wave propagation and fluid dynamics" (V. Michel-Dansac, E. Franck)
- PostDoc Leopold Tremant, 2023-2024, "Structure preserrving ML for ODE" (C. Courtès, E. Franck, L. Navoret)
- PostDoc Youssouf Nasseri, 2023-2024, "data driven reduced models for Vlasov equations" (C. Courtès, E. Franck, L. Navoret)
- PhD Thesis Roxana Sublet, 2023-, “Mathematical models for collective cell dynamics”(50% L. Navoret)
- PhD Thesis Amaury Bélières-Frendo, 2023-, "Shape optimization through learning" (25% V. Michel-Dansac)
- PhD Thesis Daria Hrebenshchykova, 2024-, "Building physics-based multilevel surrogate models from neural networks. Application to electromagnetic wave propagation" (33% V. Michel-Dansac)
- PhD Thesis Nicolas Pailliez, 2024-, "Implicit neural representation and opertator learning for multi-scale physical problems" (V. Michel-Dansac, E. Franck, L. Navoret)
- PhD Thesis Virgile Bertrand, 2024-, "Constructing the structural method for hyperbolic partial differential equations" (33% V. Michel-Dansac, 33% E. Franck)
- PhD Thesis Guillaume Steimer 2021-, "Hamiltonian data driven reduced models" (25% L. Navoret, 25% E. Franck, 25% V. Vigon)
- PhD Thesis Mei Pallanque 2022-, "New models for radiative transfer in reionization" (30% E. Franck)
- PhD Thesis Frédérique Lecourtier 2023-, "Hybrid ML and finit element methods for digital twins" (33% E. Franck)
- PhD Thesis Killian Lutz 2023-, "Control for quantum system" (50% E. Franck)
- PhD Thesis Claire Schnoebelen 2023-, "Sructure presering ML methods for symplectic PDEs" (33% E. Franck, 33% L. Navoret)
- PhD Thesis Lauriane Turelier, 2023- (50% C. Courtès)
- PhD Thesis Hassan Ballout 2024-, (33% J. Aghili)
- PhD Thesis Clément Flint, 2020-2024, (50 % P. Helluy)
- PhD Thesis Gauthier Lazare, 2022-, (50 % P. Helluy)

- PhD Thesis Stéphane Dilungana, 2020-2024, "Apprentissage automatique et optimisation pour la détermination des propriétés acoustiques d'une salle à partir de signaux audio", Link (33% A. Deleforge)
- PhD Thesis Tom Sprunck, 2021-2024, "Can one hear the shape of a room ? Room Geometry Reconstruction from Acoustic Measurements using Super-Resolution and Shape Optimization" [16] (33% A. Deleforge)
- PhD Thesis Robin San Roman 2022-, "Apprentissage autosupervisé de représentations audio désintriqués pour la compression et la génération" (33% A. Deleforge)
- Master Thesis (M2) Alexis Schmitt, "Introduction to the finite element method" (V. Michel-Dansac)
- Master Thesis (M2) Jérémy Pawlus "Learning Green functions and reduced modeling for the Helmholtz equation" (V. Michel-Dansac, E. Franck, A. Deleforge)
- Master Thesis (M2) Virgile Bertrand "`ScimBa`: Combining Numerical Methods and Machine Learning for Solving PDEs" (V. Michel-Dansac, E. Franck)
- Master Thesis (M2) B. Gaunard, Agreg project, "Symplectic schemes" (L. Navoret)
- Master Thesis (M2) Barnabé Miesch "Réflexion acoustique en incidence oblique et estimation de l'impédance de paroi par optimisation numérique." (50% A. Deleforge)
- Master Thesis (M1) Marie Sengler, co-supervised with Thales, "Multiscale electrostatics and magnetostatics simulations on complex domains" (V. Michel-Dansac, E. Franck)
- Master Thesis (M1) Rayen TLILI, "Interfacing Feel++ and Scimba" (J. Aghili)
- Master Thesis (M1) Adama DIENG, "The Discontinuous Galerking method in 1D" (J. Aghili)
- Master Thesis (M1) Hatim Ellabib, "Micro macro modeling for radiative transfer" (E. Franck)
- Master Thesis (M1) Antoine Regardin, "Adaptive implicit methods for hyperbolic scalar equation" (A. Thomann, E. Franck)
- Bachelor Thesis (L3) Elisa Cuoco (C. Courtès)
- Bachelor Internship (L2), "development of a personal researcher webpage generator" (M. Boileau)
- Apprentice developer, IRMA information system, web projects (M. Boileau)

10.2.3 Juries

- Reviewer and jury member of the PhD defense of Davide Ferrari, February, University Trento, Italy (A. Thomann)
- Member of the selection committee for associate professors (MCF), CNU 26, University of Lorraine (C. Courtès)
- Member of the recruitment committee for an AGPR, ENS de Cachan (C. Courtès)
- Jury member for the external aggregation of mathematics (C. Courtès)
- Jury member of the mathematics olympiad of 1ère (C. Courtès)
- Jury member for the defense of projects aiming to obtain the ITI++ University Diploma (J. Aghili)
- Jury member for the recruitment of three ATER positions and Contract Teachers at UFR Maths-Info (J. Aghili)
- Member of the Inria research engineer recruitment jury, June, MIMESIS (M. Boileau)

- Member of the regional commission for ranking CNRS engineers and technicians (M. Boileau)
- President of the PhD jury of Valentin Ritzenthaler, Toulouse university (P. Helluy)
- President of the PhD jury of Camille Poussel, Toulon university (P. Helluy)
- President of the PhD jury of Anil Gün, ICUBE, Strasbourg university (P. Helluy)
- HDR warrant of L. Navoret, Strasbourg university (P. Helluy)
- Reviewer for the PhD Thesis of Wageesha Manamperi, The Australian National University, Canberra (A. Deleforge)

10.3 Popularization

10.3.1 Productions (articles, videos, podcasts, serious games, ...)

- Article: "Des modèles mathématiques pour simuler des problèmes d'ingénierie" to appear in the collective book M. Bouzeghoub, M. Daydé et C. Jutten (dir.) - Le calcul à découvert, CNRS Éditions (P. Helluy)

10.3.2 Participation in Live events

- Speed-meetings between high school girls and scientific women for the event "Sciences, un métier de femmes", March (C. Courtès)
- Scientific workshop "modelling a chocolate cake" for high school students, March (C. Courtès)
- Research talks aimed at high school students, June (C. Courtès)
- Co-organization of the mathematics and computing week "Les Cigognes" for high school girls, since 2022 (C. Courtès)
- Scientific computing workshop for middle school students during the "Semaine des Mathématiques 2024" (M. Boileau)
- 1h mediation sessions on digital science research in 7 classes of 2nd in the highschools of Bouxwiller and Bischwiller for the programm Chiche SNT (A. Deleforge)

10.3.3 Others science outreach relevant activities

- Journées des Universités et des formations post-bac, présentation des filières à l'UFR maths-info, Janvier (C. Courtès, J. Aghili)

11 Scientific production

11.1 Major publications

[1] E. Franck, V. Michel-Dansac and L. Navoret. 'Approximately well-balanced Discontinuous Galerkin methods using bases enriched with Physics-Informed Neural Networks'. In: *Journal of Computational Physics* (1st Sept. 2024). DOI: 10.1016/j.jcp.2024.113144. URL: https://hal.science/hal-04246991.

11.2 Publications of the year

International journals

[2] J. Aghili, R. Hild, V. Michel-Dansac, V. Vigon and E. Franck. 'Accelerating the convergence of Newton's method for nonlinear elliptic PDEs using Fourier neural operators'. In: *Communications in Nonlinear Science and Numerical Simulation* 140.2 (Jan. 2025), p. 108434. DOI: 10.1016/j.cnsns.2024.108434. URL: https://hal.science/hal-04440076 (cit. on p. 18).

[3] A. Bélières–Frendo, E. Franck, V. Michel-Dansac and Y. Privat. 'Volume-Preserving Geometric Shape Optimization of the Dirichlet Energy Using Variational Neural Networks'. In: *Neural Networks* 184 (Apr. 2025), p. 106957. DOI: 10.1016/j.neunet.2024.106957. URL: https://hal.science/hal-04663197 (cit. on p. 19).

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[5] W. Boscheri and A. Thomann. 'A structure-preserving semi-implicit IMEX finite volume scheme for ideal magnetohydrodynamics at all Mach and Alfvén numbers'. In: *Journal of Scientific Computing* (1st July 2024). DOI: 10.1007/s10915-024-02606-1. URL: https://hal.science/hal-04495185 (cit. on p. 15).

[6] M. Boujoudar, E. Franck, P. Hoch, C. Lasuen, Y. Le Henaff and P. Paragot. 'A composite finite volume scheme for the Euler equations with source term on unstructured meshes'. In: *ESAIM: Proceedings and Surveys* (2024), pp. 1–22. URL: https://hal.science/hal-04543142. In press (cit. on p. 17).

[7] C. Courtès, M. Boileau, R. Côte, P. A. Hervieux and G. Manfredi. 'Micromagnetic simulations of the size dependence of the Curie temperature in ferromagnetic nanowires and nanolayers'. In: *Journal of Magnetism and Magnetic Materials* 598 (24th Apr. 2024), p. 172040. DOI: 10.1016/j.jmmm.2024.172040. URL: https://hal.science/hal-04364178 (cit. on p. 19).

[8] C. Flint and P. Helluy. 'Reducing the memory usage of Lattice-Boltzmann schemes with a DWT-based compression'. In: *ESAIM: Proceedings and Surveys* 77 (18th Nov. 2024), pp. 79–99. DOI: 10.48550/arXiv.2302.09883. URL: https://inria.hal.science/hal-03990880 (cit. on p. 17).

[9] C. Flint, A. Huppé, P. Helluy, B. Bramas and S. Genaud. 'Using the Discrete Wavelet Transform for Lossy On-the-Fly Compression of GPU Fluid Simulations'. In: *International Journal for Numerical Methods in Fluids* (27th Oct. 2024). DOI: 10.1002/fld.5344. URL: https://inria.hal.science/hal-04582282 (cit. on p. 17).

[10] E. Franck, V. Michel-Dansac and L. Navoret. 'Approximately well-balanced Discontinuous Galerkin methods using bases enriched with Physics-Informed Neural Networks'. In: *Journal of Computational Physics* (1st Sept. 2024). DOI: 10.1016/j.jcp.2024.113144. URL: https://hal.science/hal-04246991 (cit. on p. 18).

[11] P. Gerhard, P. Helluy, V. Michel-Dansac and B. Weber. 'Parallel kinetic schemes for conservation laws, with large time steps'. In: *Journal of Scientific Computing* 99.1 (2024). DOI: 10.1007/s10915-024-02468-7. URL: https://hal.science/hal-03910307 (cit. on pp. 5, 16).

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Doctoral dissertations and habilitation theses

[15] L. Navoret. 'Models and numerical methods for multiscale transport problems'. Université de Strasbourg, 20th Dec. 2024. URL: https://theses.hal.science/tel-04826632.

[16] T. Sprunck. 'Can one hear the shape of a room ?: Room Geometry Reconstruction from Acoustic Measurements usingSuper-Resolution and Shape Optimization'. Université de strasbourg, 17th Dec. 2024. URL: https://hal.science/tel-04818990 (cit. on p. 33).

Reports & preprints

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[18] T. Bellotti, P. Helluy and L. Navoret. *Fourth-order entropy-stable lattice Boltzmann schemes for hyperbolic systems.* 19th Mar. 2024. URL: https://hal.science/hal-04510582 (cit. on p. 18).

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[21] S. Clain, E. Franck and V. Michel-Dansac. *Structural schemes for Hamiltonian systems.* 23rd Jan. 2025. URL: https://hal.science/hal-04911125.

[22] R. Côte, C. Courtès, G. Ferriere, L. Godard-Cadillac and Y. Privat. *Existence and Uniqueness of Domain Walls for Notched Ferromagnetic Nanowires.* 9th Dec. 2024. URL: https://hal.science/hal-04827510 (cit. on p. 20).

[23] M. Dumbser, M. Lukáčová-Medvid'ová and A. Thomann. *Convergence of a Hyperbolic Thermodynamically Compatible Finite Volume scheme for the Euler equations.* 20th Dec. 2024. URL: https://hal.science/hal-04850839 (cit. on p. 15).

[24] M. Duprez, V. Lleras, A. Lozinski, V. Vigon and K. Vuillemot. *Phi-FD : A well-conditioned finite difference method inspired by phi-FEM for general geometries on elliptic PDEs.* 10th Oct. 2024. URL: https://hal.science/hal-04731164 (cit. on p. 21).

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[26] E. Franck, I. Lannabi, Y. Nasseri, L. Navoret, G. Parasiliti Rantone and G. Steimer. *Hyperbolic reduced model for Vlasov-Poisson equation with Fokker-Planck collision.* 15th Apr. 2024. URL: https://hal.science/hal-04099697.

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[30] T. Sprunck, A. Deleforge, Y. Privat and C. Foy. *Fully Reversing the Shoebox Image Source Method: From Impulse Responses to Room Parameters.* 3rd May 2024. URL: https://hal.science/hal-04567514 (cit. on p. 21).

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