Multilevel physics informed neural networks (MPINNs)

Abstract

In this paper we introduce multilevel physics informed neural networks (MPINNs). Inspired by classical multigrid methods for the solution of linear systems arising from the discretization of PDEs, MPINNs are based on the classical correction scheme, which represents the solution of the PDE as the sum of a fine and a coarse term that are optimized in an alternate way. We show that the proposed approach allows us to reproduce in the neural network training the classical acceleration effect observed for classical multigrid methods, thus providing a PINN that shows improved performance compared to the state-of-the-art. Thanks to the support of the coarse model, MPINNs provide indeed a faster and improved decrease of the approximation error in the case both of elliptic and nonlinear equations and a more robust asymptotic behaviour.

1 Introduction

The approximation of the solution of partial differential equations (PDEs) by artificial neural networks (ANNs) dates back to the 90s (Lagaris et al., 1998), but it is only in these last years that this topic fully emerged and gave rise to a really active field of research. ANNs have been used for many different purposes in this field: for the numerical solution of either direct problems (Di Muro & Ferrari, 2008; Raissi et al., 2019; Rudd, 2013; Mishra, 2018; Sirignano & Spiliopoulos, 2018; Luo & Yang, 2020) or of inverse problems (Raissi & Karniadakis, 2018; Raissi et al., 2017b), to reconstruct the equation from given data (Long et al., 2018; Rudy et al., 2017; Schaeffer, 2017), to learn dynamics from incomplete information and physical priors (Ayed et al., 2019; De Bézenac et al., 2019). ODE solvers have even been used for supervised learning problems (Chen et al., 2018). Also the interpretation of successful ANNs like ResNET as ODE discretization schemes is an important direction (Ruthotto & Haber, 2019; Lu et al., 2018), as well as the study of the issues of stability and robustness for different schemes (Haber et al., 2019; Chang et al., 2018).

In this field, the most famous network architecture is the one of PINNs (physics informed neural networks), introduced for the first time in Raissi et al. (2019; 2017a;b). Since their introduction, the PINNs architecture has encountered a growing interest and the good performance observed in practice have been later supported by theoretical results. In Mishra & Molinaro (2020b;a) the authors propose rigorous estimates on the generalization error of PINNs approximating the solution of the direct and inverse problems for PDEs data assimilation problems in terms of the training error and number of training samples, while convergence results for the sequence of approximations to the solution of linear second-order elliptic and parabolic PDEs when the number of data grows are proposed in Shin et al. (2020).

Despite their good performance, the training of such networks may still represent a challenge in case of difficult problems, such as highly nonlinear problems. In this case really large networks may be needed to correctly represent the sought solution, leading to the need of solving a really large-scale optimization problem, for which standard training methods may show a slow convergence, and it may be difficult to properly tune the learning rate.

When dealing with linear PDEs, multigrid (MG) methods are by far the most effective methods for the solution of large scale problems (Hackbusch, 1985; Briggs et al., 2000; Trottenberg et al., 2000). The improved performance of MG methods derives from the fact that alternating relaxations among

fine and coarse grids allows us to more efficiently reduce all the components of the error, smooth and oscillatory ones.

The same behaviour can be observed in multilevel optimization for nonlinear problems (Gratton et al., 2008; Groß & Krause, 2009; Kočvara & Mohammed, 2016; Lewis & Nash, 2005; 2013; Nash, 2000; 2014; Wen & Goldfarb, 2009; Calandra et al., 2021), which still exploits representations of the problem at different scales. If in MG methods the residual of the nonlinear equation is transferred from a grid to the other, in such schemes the variables of the optimization problems are the object of the transfer operators. It is evident then that the application of such techniques to neural network training is not straightforward, as the transfer operators usually used in MG and multilevel optimization (standard interpolation and restriction operators) requires the quantities that need to be transferred to possess an underlying geometrical structure in order to be effective. In the case of a training problem, the variables subject to optimization are the weights and biases of the network, which do not possess any geometrical structure. To derive a multilevel method for the training problem, it is then necessary to design multilevel transfer operators differently and it is not evident how to do that.

Previous contributions have been made in this direction in Calandra et al. (2020). The authors propose a strategy to transfer the weights that is inspired to algebraic multigrid (Ruge & Stüben, 1987; Brandt, 2000), which however requires the knowledge of the Hessian matrix of the loss function, which is impractical for really large scale problems. Moreover the proposed approach is designed for one layer neural networks, which limits the range of applications of the approach.

In this work we avoid this problem by following a completely different path: diverging from classical multilevel optimization methods and remaining closer to MG methods, we propose a multilevel PINN approach (MPINN), based on writing the solution of the PDE as a sum of two terms, a fine and a coarse one. Each term is a PINN depending on a different number of parameters and trained on a different training set, which are optimized independently the one from the other, as each PINN has its own weights and training points that are not transferred from a network to the other one. As in classical MG, the method proceeds by alternating relaxations on the two levels, which in this case are epochs of training of each PINN. As it is common in the multilevel literature, the approach is presented in the two-levels framework, but by a recursive scheme it can be naturally extended to the multilevel case. In such case, the solution of the PDE will be written as the sum of a finite number of increasingly coarser networks. Interestingly, this approach allows us to reproduce the acceleration typically observed in classical MG methods, in the context of the training of PINNs, as we show in the numerical results.

Related work The idea of exploiting multiple scales in learning is not new. We mention for instance Haber et al. (2018); Ke et al. (2017) that propose multiscale methods for convolutional neural networks, which connect low-resolution and high-resolution data through prolongation and restriction of CNN parameters or shallow and deep networks, leading to new training strategies that gradually increase the depths of the CNN while re-using parameters for initializations.

A similar idea is employed in Cai & Xu (2019), but in the context of partial differential equations. Multi-scale deep neural networks are introduced, based on specific techniques to convert the learning or approximation of high frequency data to that of a low frequency ones. Still in this context, Fan et al. (2019) introduce neural networks with a novel multiscale structure inspired by hierarchical matrices, which are used to approximate discrete nonlinear maps obtained from discretized nonlinear partial differential equations, such as those arising from nonlinear Schrödinger equations.

In Chung et al. (2017) the authors propose hierarchical multiscale recurrent neural networks, that can capture the latent hierarchical structure in temporal sequences by encoding the temporal dependencies with different timescales.

With respect to these methods, our is closer in spirit to classical multigrid and enables at the same time a multilevel structure in the space of the network's parameters and in that of the samples.

Structure of the manuscript The manuscript is organised as follows. In Section 2 we briefly review the standard PINNs architecture and in Section 3 the standard multigrid method. Section 4 represents the main contribution of this work, where we introduce the multilevel PINNs. In Section 5, we show numerical evidence of the advantage of the MPINNs over classical PINNs, showing

in particular that we are able to achieve, thanks to the two-levels structure, the acceleration effect classically observed in multigrid methods. Conclusions and perspectives are presented in Section 6.

2 PHYSICS INFORMED NEURAL NETWORKS

PINNs (Raissi et al., 2019) are neural networks that are trained to approximate the solution $u(z)$ of a partial differential equation. To do that, a loss function is defined that is composed of two terms, a term taking into account the physical information and a data-fidelity term.

Consider for instance a stationary PDE written as:

$$D(z, u(z)) = f(z), \; z \in \Omega, \tag{1a}$$
$$B(z, u(z)) = f_B(z), \; z \in \partial\Omega, \tag{1b}$$

where $\Omega \subseteq \mathbb{R}^d$, $d \geq 1$, is a connected subset, $\partial\Omega$ is the boundary of Ω, D is a differential operator, B is an operator defining the boundary conditions, and $f, f_B : \mathbb{R}^d \to \mathbb{R}$ are given functions.

For problem equation 1 the loss function reads as:

$$\mathcal{L}(p) = RMSE_{res}(p) + RMSE_{data}(p) \tag{2a}$$
$$RMSE_{res}(p) = \frac{\lambda^r}{N^r} \|D(z, \hat{u}_N(p; z^r)) - f(z^r)\|^2, \tag{2b}$$
$$RMSE_{data}(p) = \frac{\lambda^m}{N^m} \|\hat{u}_N(p; z^m) - u(z^m)\|^2, \tag{2c}$$

where z^r is a vector of N^r sample points in Ω in which the residual of the PDE is evaluated and z^m is a vector of N^m sample points in $\Omega \cup \partial\Omega$ in which the values of the solution are known; λ^r, λ^m are weights to balance the two components and $\hat{u}_N(p; z)$ is the sought approximation, which during training is a function of p, the set of N weights and biases. Notice that training a PINN does not require the discretization of the operator D, as $D(\hat{u}_N(p; z))$ can be directly computed, for instance by backpropagation.

Once the PINN is trained, we have at our disposal the desired approximation $\hat{u}_N(p^*; z)$ to $u(z)$. The approximation depends on the number of parametres used to parametrize the network, N, which is a parameter fixed before the training.

3 CLASSICAL MULTIGRID METHODS

In this section we briefly review the basic idea behind classical multigrid (MG) methods (Hackbusch, 1985). Consider a linear system arising from the discretization of a PDE:

$$Au = f.$$

Assume to have at disposal some approximation v to the exact solution. There are two important measures of v as an approximation to u. One is the error (or algebraic error) and is given simply by $e = u - v$, which is however just as inaccessible as the exact solution itself. However, a computable measure of how well v approximates u is the residual, given by $r = f - Av$. The residual is simply the amount by which the approximation v fails to satisfy the original problem $Au = f$. Assuming that the solution of the linear system is unique, we have $r = 0$ if and only if $e = 0$ (however, it may not be true that when r is small in norm, e is also small in norm). Using the definitions of r and e, we can derive the so-called *residual equation*, an extremely important relationship between the error and the residual:

$$Ae = r.$$

The residual equation is used in multigrid methods to great advantage. Given the approximation v, it is easy to compute the residual. To improve the approximation v, we might solve the residual equation for e and then compute a new approximation using the definition of the error $u = v + e$. Usually a relaxation scheme is used to solve the linear systems. Many relaxation schemes possess the so called *smoothing property*, meaning that they are efficient in eliminating the oscillatory modes of the error, while they tend to leave the smooth ones. This is a limiting property of relaxation methods, which is corrected by multigrid methods thanks to this key observation: passing from a

fine grid Ω_h to a coarse grid Ω_H, a mode becomes more oscillatory. The relaxation method will then efficiently remove the oscillatory components of the error if used on a coarse grid. Mutigrid methods then obtain really good speed ups by alternating relaxations among fine and coarse grids. The main scheme of MG is the following. Assume to have discretized the problem with two different resolutions, obtaining two subproblems: a fine one $A_h u_h = f_h$ and a coarse one $A_H u_H = f_H$, and assume to have at disposal two linear operators R (restriction) and P (prolongation) to transfer information from a grid to the other one. A V-cycle of MG on two levels follows the following scheme:

- Relax ν_1 times on $A_h u_h = f_h$ to obtain an approximation v_h
- Compute the residual $r_h = f_h - Av_h$.
- Project the residual on the coarse level $r_H = Rr_h$
- Relax ν_2 times on the residual equation $A_H e_H = r_H$ to obtain e_H
- Correct the fine level approximation $v_h = v_h + e_h$, where $e_h = Pe_H$.

This procedure is the basis of what is called the *correction scheme*. Having relaxed on the fine grid until convergence deteriorates, we relax on the residual equation on a coarser grid to obtain an approximation to the error itself. We then return to the fine grid to correct the approximation first obtained there. Multiple V-cycles can be performed and in case of more than two levels the procedure can be extended in a recursive way. It is well-known that multigrid techniques outperform standard Gauss Siedel method and already two-grid algorithm can result in tremendous reduction in the iteration count (Mazumder, 2016).

4 MULTILEVEL PINNS

Inspired by classical MG, we write the solution of our problem as the sum of two terms:

$$\hat{u}_h(p_h; z_h) + \hat{u}_H(p_H; z_H),$$

where $\hat{u}_h(p_h; z_h)$ corresponds to the "fine" term and is a PINN parametrized by h weights and biases and trained on a fine set z_h of samples, which has enough expressive power to correctly approximate the solution of the PDE, while $\hat{u}_H(p_H; z_H)$ corresponds to the "coarse" term and is a PINN parametrized by $H < h$ parameters and trained on a coarse set of samples z_H, which is not expressive enough for the problem at hand.

The training is inspired to the classical multigrid scheme, which alternates relaxations at coarse and fine level. If we assume that D is linear and that $\lambda^m = 0$, we can recover exactly the classical MG scheme. We define the fine and coarse problems as follows:

$$\min_{p_h} \mathcal{L}_h(p_h) = \frac{1}{N_h^r} \| D(z_h^r, \hat{u}_h(p_h; z_h^r)) - f(z_h^r) \|^2, \tag{3}$$

$$\min_{p_H} \mathcal{L}_H(p_H) = \frac{1}{N_H^r} \| D(z_H^r, \hat{u}_H(p_H; z_H^r)) - r(z_H^r) \|^2. \tag{4}$$

The training in this case follows the following scheme:

- Perform ν_1 epochs on problem equation 3 to obtain an approximation $\hat{u}_h(p_h, z)$ of $u(z)$
- Compute the residual $r_h(z_h^r) = f(z_h^r) - D(z_h^r, \hat{u}_h)$
- Project the residual on the coarse level $r_H = R(r_h)$
- Perform ν_2 epochs on the residual problem equation 4 to obtain $\hat{u}_H(p_H, z)$
- Correct the fine level approximation $\hat{u}_h(p_h, z_h) + P(\hat{u}_H(p_H, z_H))$.

The main difference between MG and this approach lies in the definition of the transfer operators R and P. In MG they are linear operators, usually standard interpolation (P_{MG}) and full-weighting restriction (R_{MG}), which are directly applied to the variables of the problem. In this case instead of

applying the operators to the variables of the optimization problem p, the parameters of the network, we apply them to the underlying geometrical variable z, and thus we define:

$$R(\hat{u}_h(p_h, z_h)) := \hat{u}_H(p_H, R_{MG}z_h)) \quad P(\hat{u}_H(p_H, z_H)) := \hat{u}_h(p_h, P_{MG}z_H)),$$

thus the restriction of a neural network is still a neural network, but with less parameters and that is evaluated on a smaller set of grid points.

In the most general case, we can still use this idea to design a multilevel PINN, by transferring directly the networks from one level to the other rather than the residual, and alternating the minimization at the two levels to correct the approximation at fine level by the information computed at coarse level. We therefore alternate the minimization of two different losses:

$$\mathcal{L}_h(p_h) = RMSE_{res\,h}(p_h) + RMSE_{data\,h}(p_h) \tag{5a}$$

$$RMSE_{res\,h}(p_h) = \frac{\lambda^r}{N_h^r}\|D(z_h^r, \hat{u}_h(p_h; z_h^r) + u_H(z_h^r)) - f(z_h^r)\|^2, \tag{5b}$$

$$RMSE_{data\,h}(p_h) = \frac{\lambda^m}{N_h^m}\|\hat{u}_h(p_h; z_h^m) + u_H(z_h^m) - u(z_h^m)\|^2, \tag{5c}$$

$$\mathcal{L}_H(p_H) = RMSE_{res\,H}(p_H) + RMSE_{data\,H}(p_H) \tag{6a}$$

$$RMSE_{res\,H}(p_H) = \frac{\lambda^r}{N_H^r}\|D(z_H^r, u_h(z_H^r) + \hat{u}_H(p_H; z_H^r)) - f(z_H^r)\|^2, \tag{6b}$$

$$RMSE_{data\,H}(p_H) = \frac{\lambda^m}{N_H^m}\|u_h(z_H^m) + \hat{u}_H(p_H; z_H^m) - u(z_H^m)\|^2, \tag{6c}$$

where $u_i(z) = \hat{u}_i(p_i; z)$ for $i = h, H$ is the approximation computed at the and of each cycle at fine/coarse level. Notice that at coarse level $\hat{u}_H$ is trained on a coarse set of training points z_H^m, but then the found approximation can be evaluated at a larger set of points when it is transferred to the fine level. Notice also that during the fine level training just the fine weights p_h of the fine network $\hat{u}_h$ are optimized, while $u_H(z)$ is a fixed term issued from the previous cycle. Conversely at coarse level $u_h(z)$ is kept fixed. The procedure is described in Algorithm 1.

Algorithm 1 2-levels training of PINNs

1: Input: starting weights p_h^0, p_H^0
2: **procedure** $MPINN(p_h^0, p_H^0)$
3:     Set $u_H(z) = \hat{u}_H(p_H^0; z)$.
4:     **for** i=1,2,... **do**
5:         Perform ν_1 epochs for the minimization of equation 5 yielding weights p_h^* and set $u_h(z) = \hat{u}_h(p_h^*; z)$.
6:         Perform ν_2 epochs for the minimization of equation 6 yielding parameters p_H^* and set $u_H(z) = \hat{u}_H(p_H^*; z)$.
7:     **end for**
8: **return** $\hat{u}(p_h^*, z) + \hat{u}(p_H^*, z)$
9: **end procedure**

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5 NUMERICAL RESULTS

In this section we validate the performance of the proposed MPINNs in the solution of 1D and 2D elliptical and nonlinear equations. If not differently specified, in all the tests we use ADAM as optimizer. The learning rates are experimentally tuned, and the best decreasing strategy is adopted for each network. The runs are performed using GPUs on Google Colab.

5.1 1D ELLIPTICAL EQUATION - ADAM

We consider first a 1D linear problem:

$$u''(z) - u(z) = f(z) \tag{7}$$

with $f(z) = -(\pi^2 + 1)\sin(\pi z) - (\alpha^2\pi^2 + 1)\sin(\alpha\pi z)$ with $\alpha = 3$ on the domain $\Omega = [-1, 1]$ with $u(-1) = u(1) = 0$. The solution of this problem is $\sin(\pi z) + \sin(\alpha\pi z)$.

We study the asymptotic behaviour of the MPINNs on Problem 7, that is we consider 1-hidden layer networks with an increasing number of neurons in the hidden layer. We compare a MPINN composed of a fine network with h neurons and a coarse network with H neurons, the corresponding one level PINN with one hidden layer of h neurons (PINN h) and a one level PINN with one hidden layer of $h + H$ neurons (PINN $h + H$), which have the same total number of parameters as our MPINN. The values of h, H are specified in Table 1. For each network we report mean value and standard deviation of the RMSE and of the loss over 10 runs with random starting weights. We choose $\nu_1 = \nu_2 = 5$ in Algorithm 1. All the networks are trained on a training set of 60 sample points, while the RMSE is evaluated on a finer grid of 100 points.

	(h,H)	MPINN	PINN h	PINN $h + H$
RMSE	(50,25)	1.4e-04± 4.1e-04	2.6e-04± 7.2e-04	7.5e-04± 4.6e-3
Loss		2.4e-04± 1.1e-04	5.6e-04± 3.2e-04	2.5e-04± 1.4e-3
RMSE	(200,100)	2.7e-04 ± 2.0e-04	2.3e-03± 2.8e-03	2.4e-03± 2.6e-03
Loss		1.9e-03± 1.1e-03	3.1e-03± 4.1e-03	1.1e-02± 1.7e-02
RMSE	(300,150)	4.4e-03±5.8e-03	6.4e-01±1.1e+00	F
Loss		2.3e-02± 2.0e-02	2.5e-02±2.1e-02	F

Table 1: Problem 7, $\alpha = 3$. Mean and standard deviation of the RMSE error over 10 independent runs with different initial guesses for the weights of the networks. "F" denotes a failure in the training process, that is the desired tolerance on the norm of the gradient of the loss function has not been reached within the desired number of iterations.

Results are reported in Table 1. We observe that MPINNs clearly outperform classical PINNs. Comparing MPINN with PINN h we can see the benefits of the joint training of a fine and a coarse network: the expressivity of the network increases, but this may just be due to the fact that the total number of parameters in MPINN is larger than in PINN h. We therefore compare MPINN also to PINN $h + H$, and we can again observe an asymptotic increased robustness over the standard PINNs, which for large values of the number of parameters becomes difficult to train. Indeed, when the number of parameters increase the peculiar structure of the MPINN allows to make the training process easier and as a result the network reaches a better approximation. It is clear that structuring the parameters in a clever way is more beneficial than just augmenting their number, to gain both computational time and expressivity.

Besides the increased robustness of MPINNs, another important advantage is the fact that they provide in most runs a much quicker decrease of the error and of the loss in terms both of number of iterations and in terms of floating point operations performed during training (which is computed as the number of flops required for the matrix-vector products operations during the training), cf. Figure 1.

Remark 5.1 *In the plots we have reported the losses for the different networks all in the same plot, we stress however that they are not directly comparable, as they are defined in different ways for the PINNs and MPINNs (cf. equation 2 and equation 10). The aim of the plots is to assess the development of the training and the choice of the learning rate.*

5.2 1D ELLIPTICAL EQUATION - BFGS

In the previous runs we have used ADAM as optimizer and we have focused on 1-hidden layer networks. However, the multilevel strategy can be coupled with any optimization scheme to perform the training and can be used to train deeper networks. The comparison between PINNs and MPINN yields similar results as in the previous tests. To show this we report in Table 2 the results obtained on on Problem 7 with $\alpha = 5$ by training 4-layers networks, a MPINN composed of a fine and a coarse network with h and H neurons in each hidden layer respectively, a PINN with h neurons in each hidden layer and a PINN with $\tilde{h}$ neurons in each hidden layer. The value $\tilde{h}$ has been computed so that the corresponding PINN has the same total number of parameters as the MPINN. All the networks are trained by LBFGS method. We then report in Figure 2 the plots corresponding to the choice $h = 150$, $H = 75$, $\tilde{h} = 163$.

Figure 1: Problem 7, $\alpha = 3$. Comparison of MPINN, PINN h, PINN $h + H$ for $h = 200, H = 100$. Up: loss function (left) and RMSE (right) values along the iterations for PINNs and MPINN networks. Bottom left: comparison of true solution of the PDE and approximations computed by PINN 200 and MPINN. Bottom right: evolution of the RMSE as a function of the number of floating point operations required for the training of the networks.

Figure 2: Problem 7, $\alpha = 5$, 4-hidden-layers PINN and MPINN trained by BFGS, $h = 150$. Loss function (left) and RMSE (right) values along the iterations for PINN and MPINN networks.

5.3   2D NONLINEAR EQUATION

We consider now a 2D nonlinear problem:

$$-\Delta u + \alpha e^u = f \text{ in } \Omega = [0, 1] \times [0, 1] \tag{8}$$
$$u(0, y) = 0 \, , u(1, y) = 0, \;\; \forall y \in [0, 1]$$
$$u(x, 0) = 0 \, , u(x, 1) = 0, \;\; \forall x \in [0, 1]$$

where f has been chosen in order to have the following function as exact solution:

$$u(x, y) = [\sin(\pi x) + \sin(3\pi x)][\sin(\pi y) + \sin(3\pi y)].$$

We consider again 1-hidden-layer networks and we compare MPINN, PINN h, and PINN $h + H$, all trained by ADAM. In 2D problems the effect of the size of the training set on the cost is far more important than in the 1D case, therefore we train the fine network on a grid of 484 points and the coarse one on a coarser grid of 400 points. The results of the tests are reported in Table 3.

	(h,H)	MPINN	PINN h	PINN $\tilde{h}$
RMSE	(100,50)	3.4e-3$\pm$ 4.3e-3	1.1e-2 $\pm$ 1.7e-2 (9/10)	2.2e-2$\pm$ 2.5e-2
Loss		7.5e-3$\pm$ 6.9e-3	5.2e-2$\pm$ 8.9e-2	2.3e-2$\pm$2.1e-2
RMSE	(200,100)	1.0e-3 $\pm$7.6e-4	1.2e-3 $\pm$ 6.3e-4	3.0e-3$\pm$ 2.5e-3 (9/10)
Loss		5.7e-3 $\pm$4.3e-3	1.8e-2$\pm$ 1.2e-2	1.2e-2$\pm$ 6.4e-3

Table 2: Problem 7, $\alpha = 5$. Mean and standard deviation of the RMSE error over 10 independent runs with different initial guesses for the weights of the networks. When numbers in parenthesis are reported it means that not all the 10 runs were successful, "F" means a failure in all the runs.

	(h,H)	MPINN(h,H)	PINN h	PINN $h + H$
RMSE	(30,15)	5.0e-2$\pm$ 1.6e-2	9.2e-2$\pm$ 4.1e-2	5.3e-2$\pm$ 1.0e-2
Loss		1.2e-1$\pm$ 3.5e-2	5.6e-1$\pm$4.7e-1	1.3e-1$\pm$ 4.0e-2
RMSE	(100,50)	3.3e-2$\pm$ 1.1e-2	4.4e-2 $\pm$1.8e-2	2.2e-1$\pm$ 3.9e-1
Loss		2.8e-2$\pm$9.3e-3	6.8e-2$\pm$ 1.2e-2	2.8e-1$\pm$4.8e-1
RMSE	(200,100)	3.0e-2$\pm$ 2.0e-2 (8/10)	4.8e-2$\pm$2.9e-2 (8/10)	F
Loss		5.0e-2$\pm$4.4e-2	1.e-1$\pm$8.6e-2	F
RMSE	(300,150)	3.0e-2$\pm$1.0e-2 (7/10)	F	F
Loss		5.0e-2$\pm$ 4.4e-2	F	F

Table 3: Problem 8, $\alpha = 0.1$. Mean and standard deviation of the RMSE error over 10 independent runs with different initial guesses for the weights of the networks. When numbers in parenthesis are reported it means that not all the 10 runs were successful, "F" means a failure in all the runs.

Results are similar to the 1D case, the increased robustness of the MPINNs compared to PINNs is visible also in these tests. We report the details of a run corresponding to $h = 10$ in Figure 3. We plot the evolution of the RMSE in terms of iterations (left) and in terms of operations (right). For the MPINN the number of operations takes into account both the operations performed at fine and at coarse level. We can see that even for a very small architecture MPINN is really competitive with respect to standard PINNs, especially in terms of operations. This gives an idea of the expected gain in the computational time, as the current implementation of MPINNs is not optimized and thus it does not allow us to directly compare the computational time.

Figure 3: Problem 8. RMSE with respect to number of iterations (left) and number of operations (right).

5.4 BURGER'S EQUATION

Burgers' equation is a fundamental partial differential equation occurring in various areas of applied mathematics. For a given field $u(x, t)$ and diffusion coefficient ν, the general form of Burgers' equation in one space dimension is the dissipative system:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}. \tag{9}$$

We have conducted preliminary tests on this equation, cf. Table 4. As in the other cases, MPINN can reach solution approximations of accuracy comparable to those obtained by classical PINNs,

but performing far less operations. We consider here PINNs with 3 hidden layers. We compare a MPINN composed of a PINN with 20 neurons and a PINN with 10 neurons in the hidden layers, and two standard PINNs with 40 and 30 neurons in the hidden layers. The PINNs are trained on a training set of 40 spatial points and 120 temporal points. The MPINN uses 80 time points on the coarse grid. The decrease of the RMSE as a function of the number of operations is depicted in Figure 4 (left). On the right, where we report the RMSE along some iterations, we can observe the effect of the coarse iterations in details. We distinguish in red the RMSE obtained after a set of 5 coarse iterations, and in blue the one obtained after a set of 5 fine iterations. We can see that the coarse iterations really help to make the RMSE decrease faster.

	MPINN	PINN 40	PINN 30
RMSE	1.5e-1±3.4e-2	1.8e-1± 2.3e-2	1.8e-1± 1.5e-1
Loss	2.5e-2± 5.6e-3	7.2e-2± 9.9e-3	0.04.6e-2± 7.6e-2
Operations	1.1e10	6.7e10	3.8e10

Table 4: Problem 9. Mean and standard deviation of the RMSE error over 10 independent runs with different initial guesses for the weights of the networks.

Figure 4: Problem 9. Left: RMSE as a function of the number of floating point operations. Right: Focus on a subset of V-cycles. The blue stars mark the RMSE at the end of a fine pass in the V-cycle, while the red stars mark the RMSE at the end of a coarse pass in the V-cycle.

6   CONCLUSIONS AND FUTURE PERSPECTIVES

We have presented MPINNs, a family of multilevel PINNs, whose training is based on the standard correction scheme used by multigrid methods, state-of-the-art methods for the solution of linear elliptical equations. Miming the correction scheme we represent the solution of the PDE as the sum of a fine and a coarse networks, which are optimized in an alternate way. We show the results of tests performed on1D and 2D problems, with elliptical and nonlinear differential operators. The preliminary results show good performance of the MPINNs compared to standard PINNs both in terms of accuracy reached in the solution and in terms of operations in the training. As a meaningful future perspective we target a deeper numerical investigation of MPINNs, in particular the use of a deeper recursion scheme, as described in Appendix A.

Broader impact   The broader impact of deep learning methods for solving PDEs has been detailed in Um et al. (2021).

Reproducibility   We have included our code in the supplementary material for reproducibility.

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A APPENDIX - DEEPER MULTILEVEL SCHEMES

It is well-known that multigrid techniques outperform standard Gauss Siedel method and already two-grid algorithm can result in tremendous reduction in the iteration count (Mazumder, 2016). We have shown that very good results can be obtained by two-levels MPINNs as well.

However, as for standard multigrid, the procedure can be extended to the case of more than two levels in recursive form. This is described in Algorithm 2 where we assume to use L levels. We write $u(z) = \sum_{l=1}^{L} \hat{u}_l(p_l, z)$, with $\hat{u}_l(p_l, z)$ for $1 \leq l \leq L$ a PINN depending on a set p_l of l parameters and trained on training sets z_l (in the algorithm we assume for simplicity that $z_l^m = z_l^r := z_l$), and we assume that for both the parameters set and the samples sets the dimension increases with l (1 is the minimum level). At each level l, ν_l training iterations are performed on the network l with the

following loss:

$$\mathcal{L}_l(p_l) = RMSE_{resl}(p_l) + RMSE_{datal}(p_l) \tag{10a}$$

$$RMSE_{resl}(p_l) = \frac{\lambda^r}{N_l} \| D(z_l, \hat{u}_l(p_l; z_l) + \sum_{i=1, i \neq l}^{L} u_i(z_l)) - f(z_l) \|^2, \tag{10b}$$

$$RMSE_{datah}(p_l) = \frac{\lambda^m}{N_l} \| \hat{u}_l(p_l; z_l) + \sum_{i=1, i \neq l}^{L} u_i(z_l) - u(z_l) \|^2. \tag{10c}$$

Algorithm 2 V-cycle of MPINNs with L levels (recursive form)

1: Input: level number l ($1 \leq l \leq L$, 1 is the minimum level), starting values of the networks parameters p_i, $i = 1, \ldots, L$
2: **procedure** $p_l, u_l(z) = MPINN(l, p_i \;\; i = 1, \ldots, L)$
3:     **for** $i = 1, \ldots, L, i \neq l$ **do** set $u_i(z) = \hat{u}_i(p_i, z)$
4:     **end for**
5:     Iterate ν_l times to minimize equation 10 to obtain p_l^*
6:     Set $p_l = p_l^*$
7:     **if** $l = 1$ **then return** $p_1, u_1(z)$
8:     **else**
9:         $p_{l-1}, u_{l-1}(z) = MPINN(l-1, p_i \;\; i = 1, \ldots, L).$
10:         Set $\hat{u}(z) = \hat{u}_l(p_l; z) + \sum_{i=1, i \neq l}^{L} u_i(z).$
11:     **end if**
12: **end procedure**

The numerical investigation of this framework is left as a meaningful future research perspective.