Multidisciplinary Iterative Neural Networks for Propagating Uncertainties in Coupled Systems

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Abstract. Analyzing the effects of uncertainties on complex multidisciplinary and coupled systems is a challenging problem when high-fidelity mathematical models of such systems are expensive to evaluate. Surrogate modeling methods can be used to overcome the computational challenge. However, most surrogate methods cannot be scaled to large-scale multidisciplinary systems or they do not resolve the coupling between disciplines. This paper proposes a novel surrogate modeling methodology called multidisciplinary iterative neural networks (MINNs). The proposed approach consists of replacing discipline models with neural network models that are trained using an iterative procedure to couple the networks. The MINNs approach is characterized using an analytical two-discipline multidisciplinary problem. The trained models are used to perform uncertainty propagation and analyze the sensitivity of one discipline to the other. The results demonstrated that the MINN formulation can achieve less than 1% prediction error for the coupling variables and their summary statistics. The MINN formulation requires approximately an order of magnitude lower evaluations of the original model as compared to direct quasi-Monte Carlo simulations. These results demonstrate that MINNs are an attractive approach for propagating uncertainties through multidisciplinary systems.

Keywords: Neural networks · Multidisciplinary design analysis · Uncertainty propagation · Sensitivity analysis.

1 Introduction

Modern complex systems are inherently multidisciplinary and coupled in nature. For example, analyzing aeroelastic effects in aircraft wings requires a coupled

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multidisciplinary design analysis (MDA) involving aerodynamics and structural calculations [3]. These systems are described by a coupled system of equations that are typically solved using methods such as fixed point iteration [9]. An aircraft wing may also have uncertain operating conditions or uncertain geometry, which will affect the performance of the wing [23]. It is necessary to analyze and quantify the effects of uncertainties. However, it is prohibitive to perform such an analysis due to the computationally expensive nature of coupled analyses required for these multidisciplinary systems.

To alleviate the computational burden of uncertainty quantification (UQ) in MDA, surrogate models or machine learning methods have been actively used. Chaudhuri and Wilcox [4] utilized Kriging surrogate models to create an uncoupled system of surrogate models to propagate uncertainties from inputs to discipline outputs. Balani et al. [1] developed a surrogate-based uncertainty quantification approach for the multidisciplinary analysis of an aircraft geometry in transonic flow. The surrogate-based approach utilizes Kriging models [15] and proper orthogonal decomposition combined with interpolation [20] to compute the quantities of interest. On the other hand, the work done by Berthelin et al. [2] developed an approach that creates a surrogate model for each discipline and resolves the coupling between the disciplines using the surrogate models. However, it is necessary to implement a modified training procedure for this approach, which requires generating samples of coupling variables to create the discipline-level surrogate models. Additionally, uncertainty quantification was not performed in this study. Furthermore, the previously mentioned modeling approaches utilize Gaussian Process (GP) models, which lack scalability to higher dimensions and large-scale problems [21].

Another recent approach developed by Dikshit et al. [5] proposed the use of discipline-level neural network models that are uncoupled and predict the final converged coupling variables of a multidisciplinary wing analysis. The authors utilized this approach to perform multidisciplinary uncertainty analysis for a wing geometry in subsonic flow. While the approach was successful, it lacked information about the coupling between the disciplines, which is an important aspect in multidisciplinary systems.

Introducing information about the coupling can significantly enhance the analysis of uncertainties in multidisciplinary systems. The information of the coupling can be used to track the effects of uncertainties from one discipline on another. This will elucidate the propagation of uncertainties through large-scale multidisciplinary systems and the sensitivity of one discipline on another. This has not been well explored in previous works on multidisciplinary uncertainty propagation and previous approaches also do not fully enable this sensitivity analysis and uncertainty tracking.

To overcome the various gaps in previous approaches, this work proposes multidisciplinary iterative neural networks (MINNs), a novel approach to modeling multidisciplinary systems using neural networks. To the best of the authors' knowledge, this is the first neural network approach that utilizes an iterative formulation to enable modeling of coupled systems using discipline-specific neural

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networks. The MINNs formulation consists of a neural network model that replaces each expensive-to-evaluate model of a discipline within an MDA. The neural networks are then trained iteratively to allow the networks to mimic the solution process for a coupled system while improving the prediction of the system through iterative refinement [6]. Once the models are trained, they are utilized in a quasi-Monte Carlo simulation (QMCS) approach to perform uncertainty analysis.

This formulation has several advantages. First, by forcing the neural networks to predict a value close to the converged coupling variables, convergence of the MDA can be enhanced as the initial solution is close to the converged values, and the iteration enforces the coupling between networks rather than locating the solution from a poor initial estimate. Second, the MINNs formulation does not require the generation of samples in the coupling variable space since the only required information is that of the converged coupling variables. Finally, it maintains the coupling between the disciplines and ensures that the outputs of the discipline-specific neural network models are consistent.

The approach proposed in this work is characterized using the Sellar problem [25], which is an analytical multidisciplinary problem that acts as a simple testbed for new multidisciplinary approaches. The prediction accuracy of the MINNs formulation is compared with a modeling approach that consists of decoupled neural networks modeling each of the disciplines, similar to the approach used in [5].

The remainder of the paper is structured as follows. Section 2 introduces the novel MINNs formulation that is proposed in this work. Section 3 describes the benchmarking method used to characterize the MINNs framework. Section 4 outlines the numerical experiments performed to characterize the MINNs approach. Finally, Sec. 5 outlines the main conclusions of this work.

2 Multidisciplinary Iterative Neural Networks

In this section, the novel neural network formulation proposed in this work for MDA is described. This novel formulation will be referred to as multidisciplinary iterative neural networks (MINNs). The formulation consists of two neural networks that model individual disciplines within an MDA. The formulation presented in the current work accounts for two disciplines. However, future work can extend this framework to more than two disciplines. An iterative neural network procedure is used to couple the two models to conduct an MDA. An overview of iterative procedures for neural networks can be found in [6]. This novel formulation allows efficient computations for multidisciplinary systems while maintaining the coupled nature of these systems. An overview of the MINN formulation is given in Fig. 1.

2.1 Mathematical Definition

To mathematically describe the MINN formulation, consider two neural networks, f_θ and g_ψ, that are defined in a coupled and iterative sense as

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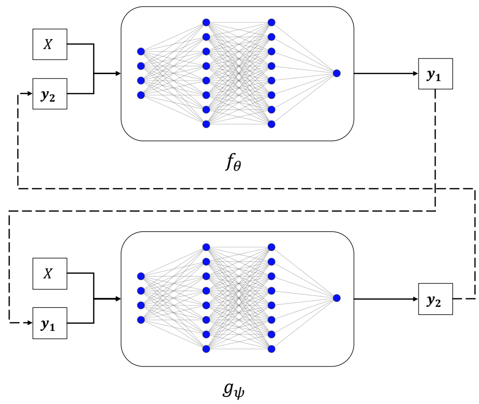

Fig. 1: Graphical overview of the multidisciplinary iterative neural networks (MINNs) framework.

$$\mathbf{y}_1^i = f_\theta(\mathbf{x}, \mathbf{y}_2^{i-1}), \quad \mathbf{y}_2^i = g_\psi(\mathbf{x}, \mathbf{y}_1^{i-1}), \quad i = 1, ..., n \tag{1}$$

where n is the total number of iterations, $\mathbf{x}$ is the input data, $\mathbf{y}_1^i$ is the value of the coupling variables from the first discipline at the i^{th} iteration, and $\mathbf{y}_2^i$ is the value of the coupling variables from the second discipline at the i^{th} iteration. The notation f_θ indicates that the neural network f is parameterized by parameters given by θ. Defining the neural networks in this manner allows for using a neural network model for each discipline while resolving the coupling between the two disciplines. This formulation requires an initial value for the coupling variables to start the iterative process. In this work, zero is used as the initial value, i.e., $\mathbf{y}_1^0 = 0$ and $\mathbf{y}_2^0 = 0$. The iterative process of the neural network prediction is continued until the absolute difference between the coupling variables of the current iteration and the previous iteration is below a specified tolerance.

2.2 Training and inference algorithm

The full training procedure of the neural networks in the MINN formulation is shown in Algorithm 1. In each epoch of training, the iterative procedure of MINNs is carried out, and the output from the neural networks at each iteration and the converged coupling variable values are used to calculate a loss function. The mean squared error loss function is used in this case. The total loss is the sum of the loss function values at each iteration. This ensures that at each iteration, the neural networks are trying to drive their output closer and closer to the converged coupling variable values. Ensuring that the neural networks also drive the value of the first iteration close to the converged coupling variables

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Algorithm 1 Training procedure for MINNs.

Require: data set of inputs and coupling variables $(\mathbf{X}, \mathbf{y}_1, \mathbf{y}_2)$, number of epochs E, convergence tolerance, $\Delta = 10^{-5}$, maximum number of iterations, M

for epoch = 1 to E **do**
  Set $\mathbf{y}_1^0 = 0$ and $\mathbf{y}_2^0 = 0$
  Compute $\mathbf{y}_1^1 = f_\theta(\mathbf{X}, \mathbf{y}_2^0)$ and $\mathbf{y}_2^1 = g_\psi(\mathbf{X}, \mathbf{y}_1^0)$
  Set $\mathbf{y}_1^{prev} = 2\mathbf{y}_1^1$ and $\mathbf{y}_2^{prev} = 2\mathbf{y}_2^1$
  i = 1
  Initialize Loss = $\mathcal{L}^{MSE}(\mathbf{y}_1^1, \mathbf{y}_1) + \mathcal{L}^{MSE}(\mathbf{y}_2^1, \mathbf{y}_2)$
  while True **do**
    Compute $\mathbf{y}_1^i = f_\theta(\mathbf{x}, \mathbf{y}_2^{i-1})$ and $\mathbf{y}_2^i = g_\psi(\mathbf{x}, \mathbf{y}_1^{i-1})$
    Increase loss value, Loss = Loss + $\mathcal{L}^{MSE}(\mathbf{y}_1^i, \mathbf{y}_1) + \mathcal{L}^{MSE}(\mathbf{y}_2^i, \mathbf{y}_2)$
    i = i + 1
    if $v_k < \Delta$ and $u_k < \Delta \; \forall \; v_k \in |\mathbf{y}_1^{prev} - \mathbf{y}_1^i|$ and $u_k \in |\mathbf{y}_2^{prev} - \mathbf{y}_2^i|$ **then**
      break while
    end if
    if i = M **then**
      break while
    end if
    Set $\mathbf{y}_1^{prev} = \mathbf{y}_1^i$ and $\mathbf{y}_2^{prev} = \mathbf{y}_2^i$
  end while
  Compute gradient of loss function, $\nabla_\eta \mathcal{L}$ where $\eta = [\theta, \psi]$
  Compute a step of the optimizer using $\nabla_\eta \mathcal{L}$
end for

can enhance convergence since the iterative procedure starts close to predicted converged values.

Backpropagation [22] is used to calculate the gradients of the total loss with respect to the parameters of both neural network models. The adaptive moment estimation (ADAM) [14] algorithm is used to update the parameters and decrease the loss function. The iterative process of computing the outputs of the neural networks is repeated at the inference stage to obtain the predictions.

2.3 Uncertainty Propagation and Sensitivity Tracking

Once the MINN formulation has been trained, it can be used to propagate uncertainties through a coupled system and also track the sensitivity of one coupling variable to another. Since the MINN formulation is cheap to evaluate, it can be used with a QMCS approach to perform uncertainty propagation given distributions of the input variables. In this work, Sobol' sequences [26] are used to generate samples from the input distributions. The sequences are implemented using the Scipy package [29]. Once the samples are generated, the MINN formulation is used to evaluate the samples and calculate the converged coupling variables. Once the converged coupling variables are known, the summary statistics and probability density functions (PDFs) of the coupling variables can be

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determined. The PDF is calculated from the outputs using a kernel density estimate [18].

After finding the PDFs of the converged coupling variables, a global sensitivity analysis [27] is performed to uncover the effects of the uncertainty in one coupling variable over another. This is enabled by the fact that the MINN formulation resolves the coupling between the disciplines, which can be exploited to track this uncertainty through the coupling. To perform the global sensitivity analysis, Sobol' sequences [26] are used to sample from the distributions of the inputs as well as the distribution of the relevant input coupling variable. These samples are then used to calculate the first-order and total Sobol' indices to uncover the sensitivities of one coupling variable to the inputs and the other coupling variable. The samples are evaluated only once using the neural network of the relevant discipline without iteration. This is because the samples of the coupling variables represent converged values. Since the neural networks are consistent according to the coupling of the disciplines, no iteration is required to obtain the converged value of the other coupling variable.

In this work, the SALib package [11, 13] is used to perform the Sobol' sensitivity analysis. This is a unique type of analysis that is enabled by the MINN formulation, as it captures the coupling between the disciplines, and it is cheap to evaluate, which is necessary for conducting the global sensitivity analysis. This is difficult with a formulation that does not account for the coupling.

3 Benchmarking method

A direct counterpart of the MINN approach is the use of independent neural networks to model each discipline without any coupling, such as the approach in [5]. In the case of independent neural networks, there is also one neural network model created for each discipline of the problem. However, these are vanilla neural network models which take the inputs of a discipline and return the converged coupling variables directly without iteration. They are termed as independent neural networks since there is no iteration where the coupling variables are exchanged and the models are not trained simultaneously. The mathematical definition for these independent neural networks can be written as

$$\mathbf{y}_1^{conv} = t_\gamma(\mathbf{x}), \quad \mathbf{y}_2^{conv} = q_\beta(\mathbf{x}), \tag{2}$$

where t_γ and q_β are neural networks with the input as $\mathbf{x}$ and output as the converged coupling variables, $\mathbf{y}_1^{conv}$ and $\mathbf{y}_2^{conv}$. This will be used as a benchmarking method for evaluating the MINN approach, as it represents an approach for discipline-specific modeling without iteration or coupling.

4 Numerical Experiments

This section formulates the uncertainty analysis of the Sellar problem, details the experiments conducted to characterize the MINN approach and the results obtained for the experiments.

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4.1 Problem Formulation

This section formulates the uncertainty analysis problem that is used to characterize the proposed approach. The multidisciplinary Sellar problem [25] is used to characterize the MINNs formulation proposed in this work. The Sellar problem consists of two coupled disciplines, and the system has three input variables. The system can be represented using the XDSM [16] diagram that is shown in Fig. 2. The problem serves as a well-defined analytical benchmark to characterize a new approach for surrogate-based multidisciplinary analysis and uncertainty propagation. There are two coupling variables in the problem, y_1 and y_2, and the three input variables are x_1, x_2, and x_3. The Sellar problem model is implemented using the OpenMDAO framework [8]. In this formulation, it is considered that the input variables are uncertain and can be described by the following distributions: $x_1 \sim U[1.0, 4.0], x_2 \sim U[-2.0, 3.0], x_3 \sim U[-2.0, 3.0]$.

The aim is to propagate uncertainties from the inputs to the converged coupling variables and describe the summary statistics and PDFs of the converged coupling variables. This will be done by employing the newly proposed MINN formulation and a QMCS approach [17]. The MINN formulation will be used to replace the solver of the Sellar problem and used to predict the coupling variables for a given set of inputs. When combined with a QMCS approach, the MINN can be used to propagate uncertainties from the inputs to the outputs.

To assess the accuracy of the results of the proposed MINN approach, ground truth values of the coupling variables and statistical quantities are required. These are created by running QMCS directly on the Sellar Problem model. Sobol' sequences [26] are used to sample from the distributions of the uncertain variables. The samples are evaluated using the Sellar Problem model. After obtaining the converged coupling variables from the Sellar Problem model, the summary statistics and PDF of the coupling variables are computed using 512 samples, as this was deemed to be sufficiently converged. The approximate mean value of y_1 is 4.7056, and the approximate standard deviation is 2.5002. The approximate mean value of y_2 is 3.0751, and the approximate standard deviation is 2.4528. These will be used as the ground truth when characterizing the proposed MINN approach in the next section.

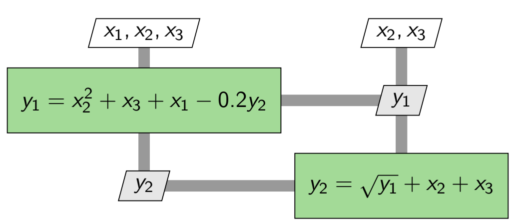

Fig. 2: Extended design structure matrix for the two discipline Sellar problem.

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4.2 Prediction accuracy of the MINN approach

The first part of this section illustrates the prediction accuracy of the proposed MINN approach. The prediction accuracy is compared with the accuracy of independent neural networks that do not account for the coupling or iteration that is included in the MINN formulation. The results presented here may slightly differ if the experiments are rerun due to randomness in the process such as randomness in the training of the neural networks.

The neural network models in the MINN formulation contain 3 hidden layers with 8 neurons each and use the sigmoid linear unit (SiLU) [7] activation function. The independent neural networks share the same architecture as the networks in the MINN formulation. However, as described previously, these independent neural networks predict the converged value of the coupling variables given a set of inputs. They do not perform any iteration or account for the coupling between the two disciplines. The results from independent neural networks will be labelled as independent in subsequent figures. All neural network models and associated tensor calculations are implemented using the PyTorch framework [19].

The normalized root mean squared error (NRMSE) metric is used to assess the accuracy of the neural networks in the MINN formulation. The NRMSE is calculated as

$$\mathrm{NRMSE} = \frac{\sqrt{\frac{1}{N}\sum_{i=1}^{N}(\hat{w}_i - w_i)^2}}{\max(w) - \min(w)}, \tag{3}$$

where N is the number of samples in the testing data, $\hat{w}$ is the predicted quantity and w are the values of the testing data. The training samples for the models are generated using Halton sequence sampling [10]. A separate set of testing data containing 100 samples is created for the models using Latin hypercube sampling [28]. Halton sequences are implemented using the Scipy package [29], and LHS is implemented using the Surrogate Modeling Toolbox [24]. The sampling bounds are chosen to correspond to the uniform distributions described in the previous section.

Figure 3 shows the variation of the NRMSE with the number of training samples for the neural network models. All plots and figures shown in this section have been created using the Matplotlib [12] and Seaborn [30] libraries. The figure illustrates that the accuracy between the MINNs formulation and the independent neural network models is comparable. Both approaches achieve similar prediction accuracy for the coupling variables when trained and tested on the same datasets. The MINN formulation achieves an NRMSE of 0.4585% and 0.5456% for y_1 and y_2, respectively, using only 60 training samples. Additionally, Fig. 4 shows the loss curves for the training process of the MINN neural network models. The figure shows two curves, one for the loss at the initial computation of the coupling variables and one for the loss after the coupling variables have converged. It is evident from the results that the value of the loss function is

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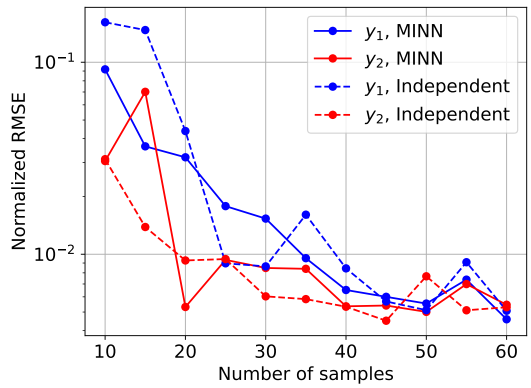

Fig. 3: Normalized root mean squared error versus number of samples for the proposed MINN approach and two independent neural networks.

much lower after convergence than at the initial computation. This confirms that the neural network outputs get closer to the true values as the iterative process continues.

While making predictions on the testing data, the MINN formulation required approximately 5 iterations on average for coupling variable convergence for an entire batch of testing data. The fixed point iteration [9] solver present within OpenMDAO [8] required approximately 7 iterations on average for convergence of the coupled equations for training data evaluations. This highlights that starting the iteration of the neural networks by predicting values close to

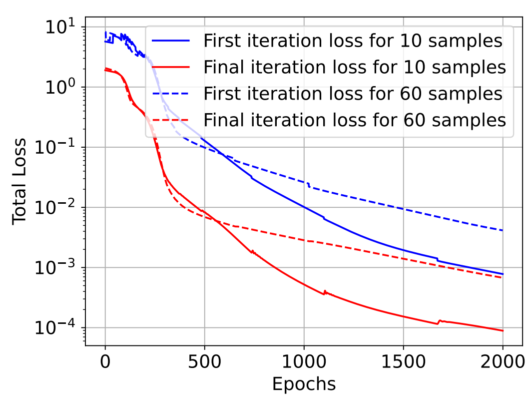

Fig. 4: Loss curves of neural networks of the MINN formulation for 10 and 60 training samples at the first and final iterations.

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the converged coupling variables can enhance overall convergence of the MDA as compared to conventional methods that do not use neural networks.

4.3 Uncertainty propagation

Using the uncertainty propagation method outlined in Sec. 2.3, the uncertainties from the input variables are propagated through the coupled system using the MINN formulation. The MINN networks trained using 60 samples are used for uncertainty propagation.

Figure 5 shows the convergence plots for the MINN formulation. The plots also show the summary statistics that were found by directly running QMCS

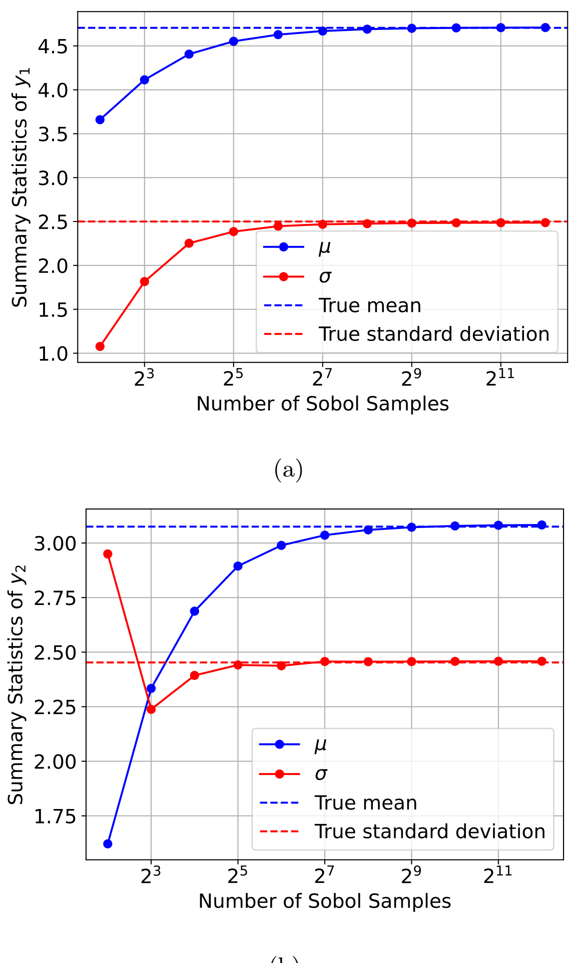

Fig. 5: QMCS convergence studies for the summary statistics of (a) y_1 and (b) y_2 using the MINN formulation.

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on the full model of the Sellar problem, and these are labeled as the true summary statistics. The plots show that the MINN formulation converges to the correct summary statistics for the Sellar problem, indicating that the approach can accurately propagate uncertainties through a coupled system. The mean and standard deviation computed using 512 QMCS samples for y_1 have a percentage difference of 0.1159% and 0.7337%, respectively, from the true values. The mean and standard deviation computed using 512 QMCS samples for y_2 have a percentage difference of 0.0911% and 0.1674%, respectively, from the true values. This shows that the summary statistics obtained from the MINN formulation only required 60 evaluations of the original model to have less than 1% error, while direct QMCS required 512 evaluations of the original model. This represents a reduction of approximately one order of magnitude in the number of evaluations required for uncertainty analysis.

Figure 6 shows the PDFs of the coupling variables that are obtained from the MINN approach and by direct QMCS on the Sellar Problem, which are labeled as the true PDFs. In both cases, the PDFs are computed using 512 QMCS samples. The PDFs obtained using the MINN formulation are a close match to the PDFs obtained directly from the Sellar Problem model. This is an expected result given the high accuracy of the MINN approach with 60 training samples.

4.4 Sensitivity analysis

Once the uncertainty has been propagated, the distributions of the converged coupling variables are known, and the MINN formulation ensures that the coupling between the disciplines is considered by the neural networks. The distribution of the coupling variable is approximated as a Gaussian distribution with the mean and standard deviation computed from the MINN networks with 512 samples. Samples are then drawn from the Gaussian distribution to perform the Sobol' sensitivity analysis.

Figure 7 shows the Sobol' indices obtained for both disciplines using the MINN formulation trained with 60 samples and the method outlined in Sec. 2.3. The results of the Sobol' analysis show that y_2 has a significant effect on the variation of y_1. It is also visible that the total Sobol' index (S_T) of y_2 is higher than the first-order index (S_1). This means that y_2 has some interactions with other variables that account for the variation in y_1. On the other hand, y_1 has a smaller effect on the variation of y_2, and the total Sobol' index is only slightly higher than the first-order index. This indicates that interactions between y_1 and other variables play a smaller role in the variation of y_2. This type of sensitivity analysis and understanding of the effects of one coupling variable on another are enabled by the MINN formulation in an efficient manner, without running the full model of each discipline.

5 Conclusion

This work proposes multidisciplinary iterative neural networks (MINNs), a novel formulation for efficiently modeling coupled multidisciplinary systems. The pro-

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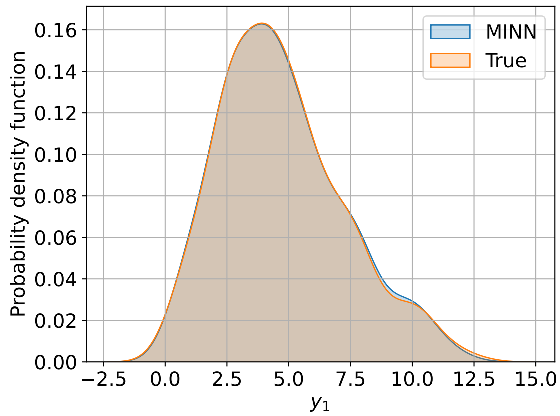
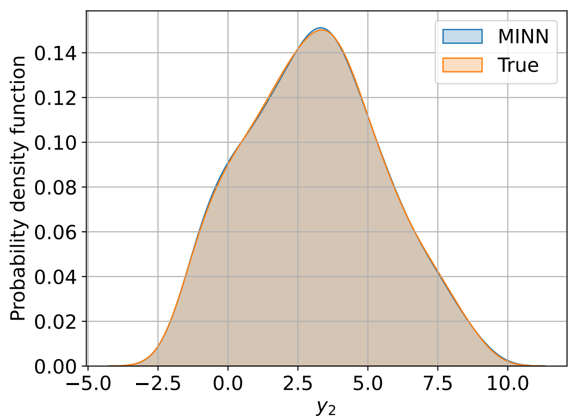


(a)



(b)

Fig. 6: Probability density functions of (a) y_1 and (b) y_2 obtained using MINN and directly from the Sellar Problem model.

posed MINN approach replaces each discipline with a cheap-to-evaluate neural network model. The neural network models are then trained using an iterative approach to ensure that the models account for the coupling between the disciplines. For the considered benchmark problem, the MINN approach shows a prediction accuracy that is comparable to training two uncoupled independent neural networks to predict the converged coupling variables directly. The MINN approach can also accurately propagate uncertainties through a coupled system, achieving results that are consistent with running QMCS directly on the full OpenMDAO [8] model. Finally, the sensitivity analysis revealed an understanding of the effects of coupling variables from one discipline on the other discipline.

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Future work will focus on extending and applying this formulation to more complex problems, such as the aerostructural analysis of wing geometries with high-fidelity simulations. This requires extending the formulation to systems with very high-dimensional coupling and input variables. Another avenue of future research will be to extend MINNs to problems with more than two disciplines.

Acknowledgments

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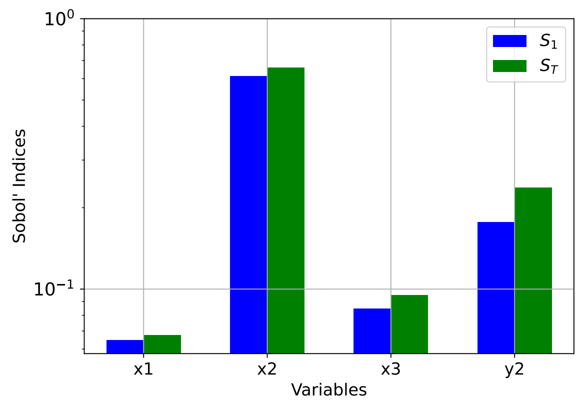
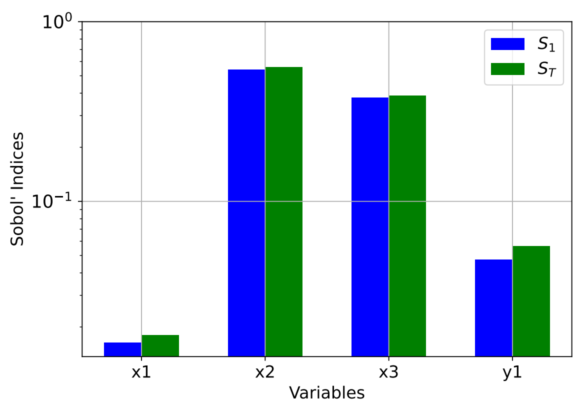


(a)



(b)

Fig. 7: Sobol' sensitivity analysis of (a) y_1 and (b) y_2 obtained using MINN and the PDFs obtained from the uncertainty analysis.

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