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Amirhossein Arzani, Kevin W. Cassel and Roshan M. D'Souza

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#### Highlights

- BL-PINN is proposed for deep learning modeling of thin boundary layers.
- BL-PINN blends classical perturbation theory in its neural network architecture.
- Accurate solution to thin boundary layers is obtained in benchmark problems.
- BL-PINN incorporates parametric dependence in its prediction without retraining.
- BL-PINN provides a hybrid PINN and reduced-physics model.

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# Theory-guided physics-informed neural networks for boundary layer problems with singular perturbation

Amirhossein Arzani<sup>a,b,\*</sup>, Kevin W. Cassel<sup>c</sup>, Roshan M. D'Souza<sup>d</sup>

<sup>a</sup>Department of Mechanical Engineering, University of Utah, Salt Lake City, UT, USA

<sup>b</sup>Scientific Computing and Imaging Institute, University of Utah, Salt Lake City, UT, USA

<sup>c</sup>Department of Mechanical, Materials and Aerospace Engineering, Illinois Institute of Technology, Chicago, IL,

USA

<sup>d</sup>Department of Mechanical Engineering, University of Wisconsin–Milwaukee, Milwaukee, WI, USA

#### Abstract

Physics-informed neural networks (PINNs) are a recent trend in scientific machine learning research and modeling of differential equations. Despite progress in PINN research, large gradients and highly nonlinear patterns remain challenging to model. This boundary layer problems are prominent examples of large gradients that commonly arise in transport problems. In this study, boundary-layer PINN (BL-PINN) is proposed to enable a solution to thin boundary layers by considering them as a singular perturbation problem. Inspired by the classical perturbation theory and asymptotic expansions, BL-PINN is designed to replicate the procedure in singular perturbation theory. Namely, different parallel PINN networks are defined to represent different orders of approximation to the boundary layer problem in the inner and outer regions. In different benchmark problems (forward and inverse), BL-PINN shows superior performance compared to the traditional PINN approach and is able to produce accurate results, whereas the classical PINN approach could not provide meaningful solutions. BL-PINN also demonstrates significantly better results compared to other extensions of PINN such as the extended PINN (XPINN) approach. The natural incorporation of the perturbation parameter in BL-PINN provides the opportunity to evaluate parametric solutions without the need for retraining. BL-PINN demonstrates an example of how classical mathematical theory could be used to guide the design of deep neural networks for solving challenging problems. Keywords: scientific machine learning, deep learning, data-driven modeling, asymptotic expansion, convective transport

<sup>\*</sup>Corresponding author

Email address: amir.arzani@sci.utah.edu (Amirhossein Arzani)

#### 1 1. Introduction

Thin boundary layers with large gradients are a common feature of high Reynolds number flows 2 and high Peclet number heat/mass transfer. The aerodynamic problem of drag reduction in turbu-3 lent boundary layers (Schoppa and Hussain, 1998), convective heat transfer in cooling (Chen et al., 4 2018), and biotransport in concentration boundary layers (Arzani et al., 2016) are a few impor-5 tant examples. Prandtl's boundary layer theory proposed during the start of the 20th century has 6 sparked continuing research in this area over the past 120 years (Erhard et al., 2010). Modeling 7 thin boundary layers is computationally challenging due to the inherently large gradients. In mo-8 mentum transport analysis, thin boundary layers in practice are typically turbulent, and therefore g numerically expensive to model. In heat and mass transport, thin boundary layers can also occur 10 in the laminar regime due to reduced diffusivity. For example, cardiovascular mass transport prob-11 lems have very thin concentration boundary layers due to the very small diffusion coefficients of 12 biochemicals in blood, which make numerical modeling very challenging (Hansen et al., 2019). 13

In recent years, data-driven modeling and scientific machine learning approaches have gained 14 considerable interest in fluid flow and transport modeling (Brunton et al., 2020; Cai et al., 2022). 15 Perhaps the earliest such work in the context of boundary layers was done by Thwaites in 1949 16 where a solution to the boundary layer momentum-integral equation was found by using a collection 17 of available experimental and analytical results to fit a term in the momentum-integral equation and 18 enable a closed-form analytical solution (Thwaites, 1949; White, 2006). The correlation method of 19 Thwaites was an early example of hybrid data-driven and physics-based modeling in fluid mechanics 20 and specifically boundary layers. 21

Physics-informed neural networks (PINN) are a trending topic in scientific machine learning and 22 enable hybrid physics-based and data-driven modeling within a deep learning setting (Raissi et al., 23 2019; Karniadakis et al., 2021). PINN has been applied to various fluid mechanics (Cai et al., 2022) 24 and heat transfer (Cai et al., 2021) problems. However, the robustness of PINN in certain problems 25 remains an issue (Karniadakis et al., 2021). PINN has limited accuracy in complex and highly 26 nonlinear flow patterns such as turbulence, vortical structures, and boundary layers (Karniadakis 27 et al., 2021). Developing robust and reliable models has been identified as a priority in scientific 28 machine learning research (Baker et al., 2019). Boundary layers are one of the topics that challenge 29 the robustness of PINNs. In current PINN models, after a sufficient reduction of the boundary layer 30 thickness (e.g., reduction in the diffusion coefficient), PINN will suffer from convergence issues. Such 31

difficulty also poses a challenge for operator learning approaches such as DeepONet (Lu et al., 2021),
which might not be able to learn parametric variations in the solution across all parameters, and
therefore robustness will be challenging to achieve.

Over the past couple of years, various variants of the original PINN approach have been pro-35 posed that attempt to overcome certain PINN limitations. Fourier feature networks have been 36 developed within PINN to overcome spectral bias in deep neural networks, which limits how well 37 high-frequency functions could be learned (Wang et al., 2021c). Conservative PINN (cPINN) (Jag-38 tap et al., 2020), extended PINN (XPINN) (Jagtap and Karniadakis, 2020), and other similar 39 domain decomposition techniques (Wang et al., 2021a) have been proposed to leverage localized 40 neural networks in regions of high gradient or complex patterns to enable efficient learning of 41 complex functions. Alternatively, other approaches have used an enhanced local sampling of the 42 collocation or training points near high gradient regions to improve convergence (Mao et al., 2020; 43 Nabian et al., 2021). However, none of these techniques studied thin boundary layers. We demon-44 strate that domain decomposition without special treatment cannot resolve the issues with learning 45 thin boundary layers due to their highly localized abrupt behavior. Additionally, we show that 46 increasing the resolution of the collocation points within the boundary layer does not resolve PINN 47 training issues. PINN has been applied to various advection-diffusion transport problems (Dwivedi 48 and Srinivasan, 2020; He and Tartakovsky, 2021; de Wolff et al., 2021; Mojgani et al., 2022) in-49 cluding boundary layers (Arzani et al., 2021; Yang et al., 2021; Bararnia and Esmaeilpour, 2022). 50 These studies investigated optimal weighting of the loss terms and mainly focused on low Peclet 51 numbers to enable a solution to these challenging problems. However, thin boundary layers (the 52 limit of vanishing viscosity/diffusivity) remain an elusive target for PINNs. 53

In this manuscript, we present a theory-guided and model-driven machine learning approach 54 for learning thin boundary layer behavior. Our framework is inspired by the singular pertur-55 bation and asymptotic expansions method for solving differential equations (Bender and Orszag, 56 1999; Van Dyke, 1975). The singular perturbation theory is a well-established approach in applied 57 mathematics and much of its developments have been inspired by the fluid dynamics commu-58 nity (O'Malley Jr, 2010). In singular perturbation problems, a small perturbation parameter (e.g., 59 viscosity in momentum transport or diffusivity in heat/mass transport) is multiplied by the highest 60 order derivative. The singular nature of the problem makes the behavior of the system in the limit 61 of vanishing perturbation very different from a zero value of the perturbation parameter. A very 62 thin boundary layer is created in such problems, and the resulting abrupt change in the solution 63

is even difficult to resolve using traditional and established numerical techniques such as the finite 64 element method (FEM) (Hansen et al., 2019). Singular perturbation solutions are tailor made 65 for such situations as they actually become increasingly accurate as the boundary layer thins and 66 the gradients increase. For example, such asymptotic basis functions have been used as the basis 67 functions in Galerkin projection in order to accurately capture and represent the singular behavior 68 inherent in such solutions (Cassel, 2019). Inspired by perturbation theory and its use as asymptotic 69 basis functions in projection methods, we propose boundary layer physics-informed neural network 70 (BL-PINN) to overcome the current limitations of deep learning in resolving thin boundary layers. 71 That is, through the lens of asymptotic expansions (Cassel, 2019), our BL-PINN approach could 72 be perceived as a PINN-driven reduced-order model (ROM) where unlike traditional ROM mod-73 els (e.g., proper orthogonal decomposition or dynamic mode decomposition) our ROM approach 74 is not data-driven but instead physics-driven. In summary, our study makes the following key 75 contributions 76

- We provide a new BL-PINN approach for physics-informed neural network modeling of thin
   boundary layers. We demonstrate in benchmark problems that our approach overcomes the
   limitations of PINN in solving forward and inverse thin boundary layer problems.
- We demonstrate how classical mathematical theories (herein, perturbation methods) could be
   replicated with PINN in a theory-guided/model-driven approach.
- Our approach provides a reduced-physics model (RPM) within PINN. This approach is entirely driven by the governing mathematical equations and is in contrast with current data driven ROM approaches, which rely on data to form their basis function. BL-PINN could be perceived as a combination of an RPM and PINN.
- Our asymptotic basis function approach in BL-PINN incorporates gauge functions (containing 86 the perturbation parameter) and the spatial coordinates dependence distinctly, and therefore 87 could be used to re-evaluate the solution as the small parameter (herein, diffusion coefficient) 88 varies. This natural incorporation of parametric dependence is an improvement compared to 89 traditional data-driven approaches. BL-PINN enables parametric PINN evaluation without 90 the need for retraining, therefore providing attractive advantages similar to operator learning 91 approaches such as DeepONet. In fact, BL-PINN actually becomes more accurate with in-92 creasing Revnolds/Peclet number, which is the opposite of traditional PINN that fails as the 93

<sup>94</sup> boundary layer thins and corresponding gradients increase.

The rest of the manuscript is organized as follows. First, we overview the solution procedure to singularly perturbed differential equations. Next, we present the BL-PINN approach along with a few benchmark problems. We present the results and demonstrate the advantage of BL-PINN over the traditional PINN approach and other variants of PINN (local clustering of collocation points and XPINN). Finally, we discuss the results and present future directions and other applications for BL-PINN.

#### 101 2. Methods

<sup>102</sup> 2.1. Problem statement: singularly perturbed differential equations

<sup>103</sup> Consider a differential equation of the form

$$L_{\epsilon} \mathbf{u} = f(\mathbf{x}) , \qquad (1)$$

subject to appropriate boundary conditions where  $\epsilon$  is a small parameter appearing in the operator 104  $L_{\epsilon}$  (e.g., a given small diffusion coefficient). We assume this is a singularly perturbed problem, which 105 means that the solution found by the differential equation when  $\epsilon = 0$  behaves very differently from 106 that in the limit  $\epsilon \to 0$ . A common scenario is when  $\epsilon$  is multiplied by the highest order derivative 107 term. This will lead to a "boundary layer" where the solution varies rapidly in a small region. 108 The thickness of this region approaches zero in the limit  $\epsilon \to 0$ . In perturbation theory (Bender 109 and Orszag, 1999; Van Dyke, 1975; Kutz, 2020), the solution to such a problem is written in terms 110 of asymptotic expansions and the solution is divided into an inner and outer region, as shown in 111 Fig. 1. The outer region (away from the boundary layer) is approximated with a regular expansion 112

$$\mathbf{u}_{\text{outer}}(\mathbf{x}) = \sum_{n=0}^{\infty} \delta_n(\epsilon) \phi_n(\mathbf{x}) , \qquad (2)$$

where  $\delta_n(\epsilon)$  are gauge functions representing the asymptotic sequence of the terms in the solution (e.g.,  $\epsilon^n$ ) and  $\phi_n(\mathbf{x})$  are functions of space that embed the solution for each order of  $\epsilon$ . As this is a regular expansion, the leading order solution corresponds to  $\epsilon = 0$ . On the other hand, to approximate the boundary layer region a stretched variable is introduced as  $\xi = \frac{\mathbf{x} - \mathbf{x}_0}{\delta(\epsilon)}$ , which allows one to zoom into the thin boundary layer region and locally represent the solution as

$$\mathbf{u}_{\text{inner}}(\mathbf{x}) = \sum_{n=0}^{\infty} \delta_n(\epsilon) \psi_n(\mathbf{x}, \epsilon) = \sum_{n=0}^{\infty} \delta_n(\epsilon) \bar{\psi}_n(\xi) , \qquad (3)$$

where  $\bar{\psi}_n(\xi)$  is the spatial function  $\psi_n(\mathbf{x}, \epsilon)$  written in terms of the stretched variable. Finally, the outer and inner solutions are matched in the overlap region using matched asymptotic expansions (Van Dyke, 1975) to obtain the final solution. Briefly, the inner solution when  $\xi \to \infty$  is enforced to match the outer solution when  $\mathbf{x} \to 0$ .

#### 122 2.2. Boundary layer physics-informed neural networks (BL-PINN)

We propose to use PINN for solving boundary layer problems with the above perturbation 123 framework, and therefore leverage the hybrid data-driven and model-driven deep learning framework 124 that PINN offers. Details about PINNs could be found in (Raissi et al., 2019). In the proposed 125 BL-PINN approach, we use separate neural networks to approximate each solution level in the outer 126 and inner expansions and use the matching condition to obtain a consistent solution. An overview 127 of the framework is sketched in Fig. 1. Multiple parallel PINNs are used to represent the different 128 orders of approximation for the inner and outer representations. Each PINN network has its own 129 physics loss function based on the PDE derived for the specified order of approximation and region 130 (inner or outer). The final solution in the inner and outer regions is derived by forming a linear 131 combination of each PINN output weighted by the known gauge functions  $\delta_n(\epsilon)$ . The final solution 132 is only used in the training process if measurement data is provided and a data loss is defined. 133 Finally, appropriate boundary conditions are imposed for each network and a matching condition 134 is used to ensure the inner and outer solutions are consistent in the overlap region between them. 135 Each neural network representing the outer layer solutions  $\phi_n(\mathbf{x})$  and inner layer solutions  $\bar{\psi}_n(\xi)$ 136 are optimized using the following loss functions 137

$$\mathcal{L}_{outer}^{n}(\mathbf{W}_{i,outer}^{n}, \mathbf{b}_{i,outer}^{n}) = \mathcal{L}_{phys,outer}^{n} + \lambda_{b} \mathcal{L}_{BC,outer}^{n} + \lambda_{d} \mathcal{L}_{data,outer} , \qquad (4a)$$

$$\mathcal{L}_{inner}^{n}(\mathbf{W}_{i,inner}^{n},\mathbf{b}_{i,inner}^{n}) = \mathcal{L}_{phys,inner}^{n} + \lambda_{b}\mathcal{L}_{BC,inner}^{n} + \lambda_{d}\mathcal{L}_{data,inner} , \qquad (4b)$$

139

138

$$\mathcal{L}_{tot} = \sum_{n} \mathcal{L}_{outer}^{n} + \sum_{n} \mathcal{L}_{inner}^{n} + \lambda_{m} \sum_{n} \mathcal{L}_{match}^{n} , \qquad (4c)$$

where n = 1, 2, ... represent the different orders of the asymptotic expansion solutions, each equipped with appropriate physics  $\mathcal{L}_{phys}^{n}$  and boundary condition  $\mathcal{L}_{BC}^{n}$  loss functions defined based on their domain (inner vs. outer) and order of approximation (n) in  $\epsilon$ . The match loss function

<sup>143</sup>  $\mathcal{L}_{match}^{n}$  is used as the matching condition for the inner and outer neural networks. The total loss  $\mathcal{L}_{tot}$ <sup>144</sup> is defined by summing the inner and outer loss functions over their order of approximation together <sup>145</sup> with the matching condition. Finally, if data is available, the data loss function  $\mathcal{L}_{data}$  is defined <sup>146</sup> and backpropogated based on the final output produced by a linear composition of all solutions as <sup>147</sup> shown in Fig. 1. The  $\lambda$  hyperparameters are set to weight the contribution of each loss term. A <sup>148</sup> standard stochastic gradient descent algorithm (Adam) is used to find the optimal weights  $\mathbf{W}_{i}$  and <sup>149</sup> biases  $\mathbf{b}_{i}$  for each layer i and each inner/outer network n.

The matching condition will require the  $\xi \to \infty$  output of the inner PINNs to match with the 150  $\mathbf{x} \to 0$  output of the corresponding outer PINNs. However, the infinity limit is not possible as neural 151 network inputs should be ideally normalized. To overcome this issue, a new variable 0 < z < 1152 is defined as  $z = \frac{\xi}{A}$  and the inner equation is rescaled using this variable. The constant A is set 153 to a sufficiently large value and  $\xi \to \infty$  is approximated as z = 1. This approach was inspired 154 by the classical similarity solutions in boundary layer theory where an appropriately large value 155 is estimated based on the equations to approximate infinity (White, 2006). Below we discuss the 156 choice of the constant A. 157

In summary, BL-PINN leverages the observation that the perturbation theory is nothing but a series of differential equations that are solved with appropriate boundary/matching conditions and the solutions are added to form the final solution. Therefore, one can use different PINN networks to solve each one of these differential equations and subsequently linearly add these predictions to form the final solution.

#### 163 2.3. Boundary layer test cases

In this section, we explain the different singular perturbation problems that were used to test the 164 proposed BL-PINN approach. In each case, BL-PINN is compared to the original PINN approach 165 (with similar network parameters). Analytical solutions or high-resolution numerical models are 166 considered as the reference for comparison. No data was used ( $\lambda_d = 0$ ) in the problems below with 167 the exception of the inverse problem (test case 5). In all of these examples,  $\epsilon$  represents a small 168 value that appears in the given equation and leads to boundary layer formation. We treat  $\epsilon$  as the 169 perturbation parameter. 100 collocation points were uniformly placed (equidistant) in the 1D and 170 2D problems producing 100 and 10,000 total collocation points, respectively. In the 3D problem 171 (test case 7), 80 points were used in each dimension producing 512,000 total collocation points. 172



Figure 1: An overview of the proposed boundary layer physics-informed neural network (BL-PINN) framework is sketched. The network architecture consists of two coupled networks: the inner and outer networks. These inner and outer regions are highlighted in a sample u(x) function shown, which exhibits a boundary layer. The inner and outer parts of BL-PINN provide an asymptotic expansion approximation to the solution in the boundary layer and outside of boundary layer regions, respectively. Each part (inner or outer) consists of multiple parallel PINN networks that each represent a certain order approximation to the solution. The final solution is derived by a combination of these parallel PINN networks. However, the final solution ( $u_{inner}$  or  $u_{outer}$ ) is not needed in the training process unless measurement data are provided and a data loss is needed. Each parallel PINN network is trained based on a PDE that is derived analytically for the desired order of approximation. The matching boundary condition (BC) loss enforces the coupling between the inner and outer networks.

#### 173 2.3.1. Test case 1: 1D linear advection-diffusion-reaction transport

First, we consider a simple 1D advection-diffusion-reaction equation presented in (Bender and Orszag, 1999; Kutz, 2020)

$$\epsilon \frac{\partial^2 u}{\partial x^2} + (1+\epsilon) \frac{\partial u}{\partial x} + u = 0 , \qquad (5)$$

where  $\epsilon$  is a small parameter set to  $5 \times 10^{-4}$ ,  $x \in [0,1]$ , and the boundary conditions are given as u(0) = 0 and u(1) = 1. Similar models known as Friedrichs' boundary layer models are commonly used to illustrate the difficulties associated with modeling viscous flow boundary layers (White, 2006). The above equation could be analytically solved, which will be used for evaluating the PINN
solution accuracy:

$$u(x) = \frac{e^{-x} - e^{\frac{-x}{\epsilon}}}{e^{-1} - e^{\frac{-1}{\epsilon}}} .$$
 (6)

An asymptotic analysis of the differential equation 5 in the limit as  $\epsilon \to 0$  reveals that the distinguished limit is  $\delta(\epsilon) = \epsilon$  based on the dominant balance between terms in the differential equation. The outer problem is then derived by substituting Eq. 2 with the gauge function  $\delta(\epsilon) = \epsilon$ into the governing equation. The leading order approximation in the outer region with  $\epsilon = 0$  (away from the boundary layer) becomes

$$\frac{\partial u_{outer}}{\partial x} + u_{outer} = 0.$$
(7)

To derive the inner problem, the gauge function  $\delta(\epsilon) = \epsilon$  is used and the stretched variable is defined as  $\xi = \frac{x}{\epsilon}$ . The leading inner problem reads

$$\frac{\partial^2 u_{inner}}{\partial \xi^2} + \frac{\partial u_{inner}}{\partial \xi} = 0.$$
(8)

The equation is rescaled to  $z = \frac{\xi}{A}$  to make the matching condition possible

$$\frac{1}{A}\frac{\partial^2 u_{inner}}{\partial z^2} + \frac{\partial u_{inner}}{\partial z} = 0.$$
(9)

The boundary conditions are  $u_{outer}(x=1) = 1$  and  $u_{inner}(z=0) = 0$ , and  $u_{inner}(z=1) = u_{outer}(x=$ 0) is the imposed matching condition. The parameter A needs to be appropriately selected. A very large parameter will create another undesirable singularly perturbed problem in Eq. 9, whereas a small parameter might not accurately represent infinity. To see how this parameter could be selected, we solve Eq. 8 to obtain  $u = Ce^{-\xi} + D$ . To approximate  $\xi \to \infty$ , we need  $e^{-\xi} \to 0$ . Selecting  $1 \times 10^{-4}$  as the tolerance leads to  $e^{-\xi} < 1 \times 10^{-4}$ , and  $\xi = 10$  is thus sufficient to represent infinity with this tolerance; therefore, A = 10 was selected.

The networks had five hidden layers with 60 neurons per layer.  $\lambda_b = 1$  and  $\lambda_m = 10$  were used, and the learning rate was  $1 \times 10^{-4}$  with 2000 epochs.

#### 198 2.3.2. Test case 2: nonlinear 1D transport problem

<sup>199</sup> A nonlinear autonomous equation is considered (Bender and Orszag, 1999)

$$\epsilon \frac{\partial^2 u}{\partial x^2} + 2\frac{\partial u}{\partial x} + e^u = 0 , \qquad (10)$$

where u(0) = u(1) = 0 are the boundary conditions and  $\epsilon = 1 \times 10^{-3}$  was used. With  $\epsilon = 0$ , the leading order outer problem is

$$2\frac{\partial u_{outer}}{\partial x} + e^{u_{outer}} = 0.$$
(11)

<sup>202</sup> The inner problem is obtained with the  $\delta(\epsilon) = \epsilon$  distinguished limit and  $z = \frac{\xi}{A}$  rescaling

$$\frac{1}{A}\frac{\partial^2 u_{inner}}{\partial z^2} + 2\frac{\partial u_{inner}}{\partial z} = 0.$$
(12)

The neural network parameters were similar to the previous problem and A = 8 was used here. The corresponding numerical simulation for comparison was performed with a fourth-order finite difference algorithm for boundary value problems (Kierzenka and Shampine, 2001). The continuation method (Vetekha, 2000) was used to enable a solution for a small  $\epsilon$ .

#### 207 2.3.3. Test case 3: 2D advection-diffusion transport in Couette flow

208 Consider the 2D advection-diffusion equation representing high Peclet number mass transport

$$u\frac{\partial c}{\partial x} + v\frac{\partial c}{\partial y} = \epsilon \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2}\right) , \qquad (13)$$

where u = 10y and v = 0 are set as the velocity components (Couette flow),  $\epsilon = 1 \times 10^{-4}$  is selected as the diffusion coefficient, and the domain is selected as  $[0,1] \times [0,1]$ . For boundary conditions,  $\frac{\partial c}{\partial y}(x, y = 0) = -10$  at the bottom wall, c = 0 at the inlet, and a no-flux Neumann boundary condition at the other boundaries is prescribed. Performing the asymptotic expansion in y gives the following leading order outer problem

$$\frac{\partial c_{outer}}{\partial x} = 0 . aga{14}$$

The leading inner problem with the distinguished limit  $\delta(\epsilon) = \sqrt{\epsilon}$ , and inner scaling  $z = \frac{\xi}{A}$  becomes

$$u(\sqrt{\epsilon}Az)\frac{\partial c_{inner}}{\partial x} = \frac{1}{A^2}\frac{\partial^2 c_{inner}}{\partial z^2} .$$
(15)

The Neumann boundary condition at the wall becomes  $\frac{\partial c}{\partial z}(x, z = 0) = -10A\sqrt{\epsilon}$ .

The neural networks had seven hidden layers with 128 neurons per layer..  $\lambda_b = 10$  and A = 8were used and the learning rate was  $5 \times 10^{-6}$  with 2000 epochs and a batch size of 128. The outer solution was simply set to c = 0 based on Eq. 14 and the boundary conditions.

Finite element method (FEM) simulation was performed in the open-source PDE solver FEniCS to provide benchmark data for comparison. The stabilized SUPG method (Brooks and Hughes, 1982) was implemented, and the mesh had 152,000 triangular elements. To facilitate convergence in the challenging high Peclet number regime, the transport model (Eq. 13) was treated as a transient problem and was integrated in time until a steady state was reached.

#### 224 2.3.4. Test case 4: 2D advection-diffusion transport in the double gyre flow

We reconsider the 2D advection-diffusion equation above (Eq. 13) with a more complicated velocity field. Namely, the double gyre flow (Shadden et al., 2005) is considered, which is a commonly used benchmark problem in chaotic advection studies (Balasuriya et al., 2018). The velocity field is defined as

$$u = -\pi B \sin(2\pi x) \cos(\pi y) , \qquad (16a)$$

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$$v = 2\pi B \cos(2\pi x) \sin(\pi y) , \qquad (16b)$$

where B = -0.1 and the domain of interest is  $[0,1] \times [0,1]$ . The diffusion coefficient is set to  $\epsilon = 1 \times 10^{-4}$ . A Neumann boundary condition with  $\frac{\partial c}{\partial y}(x, y = 0) = -10$  is imposed at the bottom wall, c = 0 is used at the left and right boundary, and zero flux is imposed on the top boundary. Similar to the previous test case, the leading order outer problem reads

$$u\frac{\partial c_{outer}}{\partial x} + v\frac{\partial c_{outer}}{\partial y} = 0.$$
(17)

The diffusion term could be kept in the outer problem to improve the solution stability. The leading order inner problem could be derived similar to test case 3 with an additional term due to non-zero vertical velocity as follows:

$$u(x,\sqrt{\epsilon}Az)\frac{\partial c_{inner}}{\partial x} + v(x,\sqrt{\epsilon}Az)\frac{\partial c_{inner}}{\partial z}/(\sqrt{\epsilon}A) = \frac{1}{A^2}\frac{\partial^2 c_{inner}}{\partial z^2} .$$
(18)

<sup>237</sup> The neural network parameters were the same as test case 3 but with a variable learning rate

between  $2 \times 10^{-4}$  and  $6 \times 10^{-6}$  during 65,000 epochs with a batch size of 256. The FEM solution was carried out similar to test case 3 but with a higher resolution mesh (318,000 triangular elements) and without stabilization.

#### 241 2.3.5. Test case 5: Inverse modeling to infer boundary flux in 2D transport

We reconsider the 2D transport problem in test case 3. We assume that the flux boundary condition at the bottom wall is unknown and use six sensors (shown in the results) to measure concentration in the boundary layer and define a data loss for inferring the unknown flux. The sensors were probed based on the FEM solution. The network parameters were set similar to test case 3 with 60000 epochs.  $\lambda_d = 10$  was used to incorporate the data measurements into the total loss.

#### 248 2.3.6. Test case 6: Axisymmetric transport in 3D Burgers vortex

In this example, we consider a 3D velocity field. The Burgers vortex is considered as a canonical vortex flow. The Burgers vortex could be derived as an asymptotic steady solution to the momentum equation and represents viscous vortices with axial stretching (Panton, 2006; Wu et al., 2007). In cylindrical coordinates  $(r, \theta, x)$ , the velocity field could be written as

$$v_r = -\frac{\gamma}{2}r\tag{19a}$$

$$v_{\theta} = \frac{\Gamma_0}{2\pi r} \left( 1 - e^{-\beta r^2} \right) \tag{19b}$$

$$v_x = \gamma x , \qquad (19c)$$

where the parameters are set to  $\gamma = 0.2$ ,  $\Gamma_0 = 2\pi$ , and  $\beta = 1$ . We consider a cylindrical domain with a radius of 0.5 and a height of x = 0.3. The diffusion coefficient is set to  $\epsilon = 1 \times 10^{-4}$  and the Neumann boundary condition at the bottom wall (x=0) is  $\frac{\partial c}{\partial x} = -5$ . Zero concentration is imposed on the side walls. Due to the symmetric nature of the transport problem, despite the 3D nature of the flow, the advection-diffusion equation could be simplified to a 2D problem in cylindrical coordinates

$$v_r \frac{\partial c}{\partial r} + v_x \frac{\partial c}{\partial x} = \epsilon \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial x^2} \right) .$$
(20)

The inner and outer problems are derived similar to test case 4. The neural network architecture was similar to test cases 3 and 4. A=8 was used and the batch size was 512. The learning rate varied between  $4 \times 10^{-4}$  and  $1 \times 10^{-5}$  with 32,000 epochs. The FEM solution was performed with a full 3D discretization (4.6M tetrahedral elements) with local boundary layer refinement.

#### 263 2.3.7. Test case 7: 3D transport near flow separation

In this example, a fully 3D mass transport problem is considered. The velocity field is defined to represent flow around a separation profile. Namely, we consider a saddle type fixed point in wall shear stress (WSS) vector field, which represents flow separation in steady flows (Surana et al., 2006). Subsequently, the velocity field near the separation point is defined using a Taylor series expansion. Such topological analysis of fluid flow has been utilized in studying flow separation (Surana et al., 2006; Wu et al., 2007) and more recently near-wall mass transport (Arzani et al., 2016; Farghadan and Arzani, 2019).

In this example, a 3D box is used to define the domain as  $[-0.7, 0.7] \times [-0.3, 0.3] \times [0, 0.3]$ . The bottom wall (z=0) is considered the separation region. The WSS vector field  $\boldsymbol{\tau}$  in this wall is defined as  $(\tau_x, \tau_y) = (-x + y, x - \frac{y}{4})$ . Subsequently, using Taylor series expansion of the WSS vector field the velocity field is extrapolated to the rest of the domain (Gambaruto et al., 2010; Arzani et al., 2016)

$$\mathbf{v}_{\pi} = \frac{\boldsymbol{\tau} z}{\mu} = \left( (-xz + yz)/\mu , \ (xz - \frac{yz}{4})/\mu \right)$$
(21a)

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$$v_z = -\frac{1}{2\mu} \nabla \cdot \boldsymbol{\tau} \ z^2 = 0.625 z^2 / \mu$$
, (21b)

where  $\mathbf{v}_{\pi} = (v_x . v_y)$  is the 2D velocity vector in the xy plane,  $v_z$  is the velocity component normal to this plane, and  $\mu$  is the dynamic viscosity set to one in this non-dimensional example. The above velocity field is used to solve the 3D advection-diffusion equation where  $\frac{\partial c}{\partial z} = -10$  is imposed at z=0 to generate a boundary layer and zero concentration is applied to the lateral walls. The inner and outer problems are derived similar to test case 4 as

$$v_x \frac{\partial c_{outer}}{\partial x} + v_y \frac{\partial c_{outer}}{\partial y} + v_z \frac{\partial c_{outer}}{\partial z} = 0$$
(22a)

v

$${}_{x}(x,y,\sqrt{\epsilon}Az)\frac{\partial c_{inner}}{\partial x} + v_{y}(x,y,\sqrt{\epsilon}Az)\frac{\partial c_{inner}}{\partial y} + v_{z}(x,y,\sqrt{\epsilon}Az)\frac{\partial c_{inner}}{\partial z} / (\sqrt{\epsilon}A) = \frac{1}{A^{2}}\frac{\partial^{2}c_{inner}}{\partial z^{2}} , \quad (22b)$$

<sup>283</sup> where the diffusion term could be brought back to the outer problem to improve stabilization, and z

in Eq. 22b is the rescaled stretched variable as defined earlier (not to be confused with the physical z coordinates in all the other equations in this Section). The network architecture was similar to previous cases (test cases 3, 4, and 6). A=8 and  $\epsilon = 1 \times 10^{-4}$  were used and a large batch size of 8192 was used to an enable efficient solution in 3D. The learning rate was varied between  $4 \times 10^{-4}$ and  $2 \times 10^{-5}$  during 24,000 epochs. The FEM simulation was performed with 2.7M tetrahedral elements with local refinement around the boundary layer region.

#### 290 3. Results

The five test case results are presented in this section. In all cases, only the O(1) networks, corresponding to the leading-order asymptotic solution, were considered in the simulations unless otherwise noted. In addition to comparison to the original PINN method for all test cases, the results are also compared to two other approaches: localized high-resolution clustering of collocation points (test case 1) and XPINN (test case 2).

The test case 1 results (linear advection-diffusion-reaction) are plotted in Fig. 2a. Observe that 296 the traditional PINN approach does not converge to a reasonable solution or capture the singular 297 boundary layer behavior near x = 0, whereas the inner and outer BL-PINN approximations match 298 the exact analytical solution very well in their respective regions. An additional original PINN 299 simulation was performed where an additional set of collocation points were seeded inside and 300 in the vicinity of the boundary layer (1000 points). The results show that this high-resolution 301 local sampling approach, which was suggested in prior work (Mao et al., 2020; Nabian et al., 302 2021), still cannot find the correct solution. In Fig. 2b, the difference between O(1), leading order 303 approximation, and  $O(\epsilon)$  approximations are shown. To distinguish between these results, case 1 was 304 repeated with a larger perturbation parameter ( $\epsilon = 0.05$ ). In this case, due to the larger diffusion 305 coefficient, the original PINN approach converges to the exact solution. In BL-PINN, increasing the 306 asymptotic expansion order does not improve the outer solution, however, the  $O(\epsilon)$  approximation 307 provides notable improvement for the inner solution. Overall, the  $O(\epsilon)$  approximation provides 308 accurate results in both inner and outer regions but does not offer any advantage over the original 309 PINN approach in this case due to the larger  $\epsilon$  value, and the correspondingly less severe gradients. 310 Test case 2 extends the previous problem to a nonlinear differential equation and also presents 311 a comparison with XPINN as shown in Fig. 3. Similar results could be seen where BL-PINN 312 approximates the true solution very well, while the original PINN approach cannot converge to the 313 correct solution. In this case, it could be seen that the original PINN approach seems to be learning 314



Figure 2: Test case 1 (linear advection-diffusion-reaction) results are plotted and the inner and outer solutions approximated by BL-PINN are compared to the original PINN approach, a high-resolution local sampling approach, and the analytical solution. a)  $\epsilon = 5 \times 10^{-4}$  and only the leading order approximation in BL-PINN is retained. b)  $\epsilon = 0.05$  and the O(1) approximation (leading order) as well as the O( $\epsilon$ ) approximation in BL-PINN are compared. PINN and analytical solutions are on top of each other in this case.

a shifted version of only the outer layer solution. The reason for the shifted solution is the imposed x = 0 boundary condition, which is where the boundary layer is occurring. XPINN cannot provide much improvement over the original PINN approach. In XPINN, the domain was decomposed into boundary layer and outer regions, and continuity was imposed at the interface. We also investigated sensitivity to the choice of the size of the boundary layer domain of XPINN and confirmed similar results (not shown).



Figure 3: Test case 2 (nonlinear advection-diffusion-reaction) results are plotted and the inner and outer solutions approximated by BL-PINN are compared to the original PINN approach, XPINN, and the true solution. The inner XPINN solution covers the very thin boundary layer region; however, it cannot discover the true solution and just continues the outer XPINN pattern based on XPINN's interface condition (continuity in solution and its flux).

The 2D advection-diffusion transport result for the Couette flow problem (test case 3) are shown in Fig. 4 and Fig. 5. The first figure shows the contour plots of the concentration results.

It could be seen that the original PINN approach does not capture the quantitative features in the boundary layer correctly, whereas BL-PINN produces results very similar to the reference FEM solution. To better visualize the quantitative features, the concentration on the bottom wall where the boundary layer is created is plotted in Fig. 5. It could be seen that BL-PINN captures the quantitative behavior much more accurately. Similar to the previous example, the original PINN solution shows a shifted behavior where in this case it predicts the qualitative trend away from x = 0 (the leading edge of the boundary layer) and only in a shifted fashion.



Figure 4: Test case 3 (2D advection-diffusion in Couette flow) contour results are shown and the BL-PINN approach is compared to the original PINN approach and the reference FEM solution.



Figure 5: Test case 3 (2D advection-diffusion in Couette flow) concentration results are plotted at the bottom wall (y = 0) where the boundary flux is imposed and the boundary layer is generated. The original PINN, BL-PINN, and reference FEM results are compared.

A more complicated advection-diffusion transport example is shown in Fig. 6 and Fig. 7 where test case 4 (double gyre flow) results are shown. The velocity vector field is sketched showing the two

counterrotating vortices in the double gyre flow. In this example, we are interested in the boundary 332 layer that forms at the bottom wall where the Neumann boundary condition is prescribed. The 333 contour results shown in Fig. 6 show that the inner part of BL-PINN is capable of capturing the 334 quantitative and qualitative behavior in the boundary layer. The original PINN approach does 335 not provide results close to the reference FEM solution (note the different color bar range). In the 336 outer region (outside of the boundary layer at the bottom wall), the problem is more complicated 337 due to the domination of advection. The BL-PINN outer network in this case cannot capture 338 quantitative concentration patterns in the outer region and only captures the qualitative behavior. 339 On the other hand, the original PINN approach completely misses the qualitative behavior and 340 cannot find even a qualitatively meaningful solution. Interestingly, the outer part of BL-PINN can 341 provide a correct quantitative approximation near the interface with the inner part of BL-PINN, 342 and therefore the matching boundary condition is satisfied, which helps produce correct boundary 343 layer results by the inner network. This is further shown in Fig. 7 where the concentration is plotted 344 at the bottom wall. We can see that BL-PINN provides a very accurate quantitative prediction of 345 the concentration pattern, while PINN cannot approximate the correct quantitative pattern. 346



Figure 6: Test case 4 (2D advection-diffusion in the double gyre flow) contour results are shown and the BL-PINN approach is compared to the original PINN approach and the reference FEM solution. In the BL-PINN panels, the entire solution is shown. However, the inner and outer solutions are only valid near and away from the bottom wall, respectively. To better demonstrate the qualitative behavior, different color bar ranges are used in some cases where the error was higher. The velocity vector field is shown on the right where normalized vector fields are superimposed on top of the streamlines to show the velocity direction.



Figure 7: Test case 4 (2D advection-diffusion in the double gyre flow) concentration results are plotted at the bottom wall (y = 0) where the boundary flux is imposed and the boundary layer is generated. The original PINN, BL-PINN, and reference FEM results are compared.

The inverse problem (test case 5) results are shown in Fig. 8. The right panel shows the placement of the measurement sensors (the six grey spheres) within the boundary layer. The left panel shows the learned flux boundary condition,  $\frac{\partial c}{\partial y}(y = 0)$ , during different epochs of the deep learning training. It is seen that BL-PINN converges to the ground truth flux that was used to generate the data, whereas the original PINN approach cannot converge to the ground truth flux.



Figure 8: Test case 5 (inverse modeling of flux in the Couette flow transport problem) results are shown on the left panel. The learned flux versus deep learning epochs are shown for the BL-PINN and original PINN approaches along with the true flux. The right panel demonstrates the location of the measurement sensors within the boundary layer that were used to define the data loss. The grey spheres mark the sensor locations

In the last two test cases (6 and 7), the BL-PINN approach did not provide accurate results in the outer region (similar to the double gyre flow problem), and therefore these results are not included. It should be highlighted that the boundary layer is the region of interest in our work, and therefore this is not a concern. In test case 7, we further substantiate this by demonstrating the success of a BL-PINN approach inspired by surface transport models where we completely omit the outer BL-PINN network in our approach. We further discuss these observations in the

Discussion. The Burgers vortex (test case 6) results are shown in Fig. 9. We can see that the BL-PINN approach leads to considerable improvement in the wall concentration results compared to the original approach.



Figure 9: Test case 6 (axisymmetric advection-diffusion in 3D Burgers vortex) results are shown. a) The BL-PINN approach is compared to the original PINN and reference FEM solution. The x=0 plane where the boundary layer forms is shown. b) The concentration results are quantitatively compared at the x=0 plane for different radial positions. c) The 3D velocity streamlines are shown in the cylindrical region of interest and are colored based on velocity magnitude.

Finally, the results for test case 7 (3D transport around flow separation) are shown in Fig. 10. 361 The original PINN cannot capture the qualitative (Fig. 10a) or quantitative (Fig. 10b) patterns. To 362 assist with qualitative visualization of the patterns, the maximum color bar range for the original 363 PINN approach is set to 0.03 and for the other approaches, this is 1.04. In this test case, we also 364 present a new BL-PINN approach where we just consider the inner network and at the matching 365 condition set zero concentration for the inner network. This approach was inspired by recent work 366 on near-wall transport in the context of biomedical flows (Hansen and Shadden, 2016; Arzani et al., 367 2016; Farghadan and Arzani, 2019) where it has been shown that in thin concentration boundary 368 layer problems one could reduce the problem to a surface transport model based on WSS and near-369 wall velocity, and therefore ignore transport away from the wall with minimal loss in accuracy for 370 most problems. Interestingly, our results here demonstrate that the BL-PINN approach with just an 371 inner network (inspired by surface transport models) produces very accurate results. As a relevant 372 note, the region of high surface concentration (red region) corresponds to the unstable manifold of 373 the WSS vector field. The unstable WSS manifold, also known as the attracting WSS Lagrangian 374 coherent structure, has been shown to dominate near-wall concentration patterns in complex 3D 375



problems (Arzani et al., 2016; Farghadan and Arzani, 2019; Arzani et al., 2017).

Figure 10: Test case 7 (3D transport near flow separation) results are shown. a) The BL-PINN approach is compared to the original PINN and reference FEM solution. Additionally, a de-coupled BL-PINN solution (just the inner network) is shown where the outer network is not included during training and is replaced with a zero concentration matching condition. In the color bar,  $c_{max}$  is 0.03 for the original PINN panel and 1.04 for the other approaches. The z=0 plane where the boundary layer forms is shown. b) The concentration results are quantitatively compared at the z=0 plane for a line passing through the middle of the plane (-0.7<x< 0.7, y=0). c) The 3D velocity streamlines are shown in the cylindrical region of interest and are colored based on velocity magnitude. Normalized velocity vectors are also plotted to show the flow direction.

#### 377 4. Discussion

In this work, boundary layer PINN (BL-PINN) was proposed for solving thin boundary layer 378 problems. One- and two-dimensional benchmark problems were presented as proof-of-concept where 379 it was shown that BL-PINN overcomes PINN limitations in solving thin boundary layer problems. 380 As illustrated here, only a small number of asymptotic basis functions is necessary to accurately 381 capture the solution using BL-PINN. This is in marked contrast to traditional numerical methods 382 that have increasing difficulty and require more small elements to capture high-gradient regions of 383 a solution. It was also shown that prior extensions of PINN (XPINN and local collocation point 384 clustering) were not able to resolve thin boundary layers. 385

Solutions of physical problems that contain large gradients give rise to numerical difficulties when solved using traditional numerical methods, such as FEM. Typically, such problems contain a parameter that becomes very small or very large, in which case perturbation methods are well suited to deciphering the solution's dependence on this parameter. Asymptotic basis functions are obtained directly from the governing differential equation. As such, they contain physical

information about how the system depends on the small or large parameter. In fact, the accuracy 391 of the asymptotic basis functions increases as the small parameter approaches zero (or the large 392 parameter approaches infinity) or as additional terms are included in the expansion. This is in 393 contrast to numerical methods attempting to capture the same solution. Their primary limitation 394 is that they only apply when the parameter is very small or large. Consequently, incorporating these 395 asymptotic basis functions into more general techniques holds great promise in combining the best of 396 both into a robust solution framework that takes advantage of the flexibility of general methods and 397 the model-driven, as opposed to data-driven, approach to capturing abrupt behavior in a solution. 398 Galerkin projection with asymptotic basis functions is one approach for accomplishing this (Cassel, 399 2019), and PINN offers an alternative framework. Such reduced-physics models (RPM) have the 400 potential to dramatically reduce the computational requirements necessary for solving physical 401 problems containing large gradients as compared to traditional numerical methods. 402

Whether for use in a projection method or PINN, the ideal basis functions would contain as 403 much information as possible about the system and accommodate solutions for a range of parameter 404 values. This is precisely what asymptotic basis functions offer. Perturbation (asymptotic) methods 405 comprise a set of techniques for obtaining the solution in terms of an asymptotic series for prob-406 lems having a very small or very large parameter. These methods allow for determination of the 407 dependence of the system of the small or large parameter in a formal manner from the governing 408 equation(s) itself without any need for data from the system. This dependence is contained in 409 the gauge functions, which unlike most ROM approaches captures the system's dependence on the 410 parameter. 411

BL-PINN shares similarities with other extensions of PINN and yet provides clear advantages 412 for boundary layer problems. Similar to XPINN and cPINN, BL-PINN is based on a domain 413 decomposition implementation of PINN where separate neural networks are used in different regions 414 and matched at the interface. However, unlike the arbitrary nature of XPINN and cPINN, BL-PINN 415 decomposes the domain into an inner region (boundary layer) and an outer region in a systematic 416 fashion inspired by the perturbation theory. Additionally, the rescaling of the equation within the 417 boundary layer enables an accurate solution to thin boundary layers, which is not possible with 418 prior approaches. Similar to the recently proposed sparse, physics-based, and partially interpretable 419 neural networks (SPINN) (Ramabathiran and Ramachandran, 2021), BL-PINN leverages rescaling 420 of the input variables to define the stretched variable  $\xi$  (similar to the mesh encoding layer in 421 SPINN) and relies on parallel neural networks and their linear combination to build the solution. 422

Therefore, similar to SPINN, BL-PINN is partially interpretable. However, BL-PINN extends 423 SPINN's interpretability since its design is based on asymptotic expansions and therefore in the 424 context of asymptotic basis functions (Cassel, 2019), BL-PINN could be interpreted as a physics-425 based reduced-order model representation with PINN where parametric dependence is naturally 426 considered in its design. In theory, defining kernels that represent boundary layer behavior (similar 427 to FEM enrichment of basis functions (Borker et al., 2017)) could be implemented in SPINN for 428 modeling thin boundary layers, however, the exponential nature of such kernels in boundary layers 420 poses a challenge for effective training of the neural networks. 430

A key advantage of BL-PINN is that it becomes more accurate as the perturbation parameter 431 becomes smaller, and therefore it is suitable for thin boundary layer problems. Interestingly, this is 432 in contrast with existing PINN methods that lose accuracy as the perturbation parameter decreases. 433 Another advantage of BL-PINN compared to other PINN approaches is its natural incorporation 434 of the perturbation parameter (e.g., diffusion coefficient) into the solution. That is, one can re-435 evaluate the solution without retraining with new parameters. In addition, BL-PINN can add 436 parallel networks as higher order approximations to the solution instead of increasing the degrees 437 of freedom in each network. Each of these higher order approximation networks is trained based 438 on a different equation and could have an arbitrary architecture independent of the other networks. 439 This could be somewhat compared to p-refinement in finite element method as opposed to an h-440 refinement analogy where one would use more collocation points. One disadvantage of BL-PINN 441 is the higher computational cost. For instance, in most examples shown in this paper, two neural 442 networks (inner and outer) were used to approximate the solution. However, similar to XPINN, 443 these neural networks could possess independent architectures and accuracy based on the region 444 of interest (inner vs outer). In terms of computational cost, BL-PINN requires at least two neural 445 networks to be trained (more networks if higher order approximation is required), and therefore has 446 roughly twice the computational cost of PINN for the same number of epochs. Nevertheless, one 447 has the freedom to reduce the outer network size to improve computational cost. For instance, in 448 the limit where the outer network is dropped (Fig. 10), BL-PINN will just need to train one neural 449 network similar to PINN. 450

An interesting observation in our results was that BL-PINN was capable of finding accurate surface concentration patterns in the boundary layer (our region of interest) even without producing necessarily accurate results in the outer region. While this might be surprising at first, our group has previously shown similar results in the context of high Peclet and high Schmidt number mass

transport problems where thin boundary layers are formed (Arzani et al., 2016; Farghadan and 455 Arzani, 2019). That is, such mass transport problems could be reduced to a surface transport 456 problem where the surface concentration patterns are determined by the WSS (a scale of near-wall 457 velocity) vector field. To further investigate this scenario, we performed a simulation in test case 7 458 where we only considered the inner neural network and at the matching interface forced the neural 459 network to be equal to zero (instead of coupling it to the outer network). This could be perceived as 460 a near-wall transport model in PINN where we are just studying transport within the boundary layer 461 and assuming the outer region to have minimal influence on the results. Interestingly, Fig. 10 shows 462 promising results for this approach where the surface concentration patterns are very similar to the 463 original BL-PINN approach. We should highlight that solving high Peclet mass transport problems 464 even with well established numerical methods such as finite element method is challenging and it 465 is not surprising to see inaccurate PINN results. For instance, various stabilization methods have 466 been proposed in the finite element literature for overcoming these numerical difficulties (Brooks 467 and Hughes, 1982; Codina, 1998; Hansen et al., 2019). 468

There are several areas where our study could be improved. Compared to the original PINN 469 approach, BL-PINN only demonstrates significant improvement once the boundary layer thickness 470 is sufficiently reduced, i.e. for small  $\epsilon$ . An example could be seen in Fig. 2b where the original 471 PINN can solve the problem due to the boundary layer size. Due to this reason, we did not present 472 thin boundary layer problems in the Navier-Stokes equations. If the momentum boundary layer 473 thickness is sufficiently reduced (Reynolds number increased), transition to turbulence will occur. 474 Therefore, special treatment of turbulence within PINN will be needed (Eivazi et al., 2021). In the 475 double gyre flow, BL-PINN could not provide quantitatively accurate concentration patterns in the 476 outer region (Fig. 6). This is a well-known problem in advection-dominated transport modeling with 477 PINN and could be improved with other approaches such as curriculum learning (Krishnapriyan 478 et al., 2021). Alternatively, a hybrid FEM-PINN approach (Mitusch et al., 2021) could be developed 479 where a traditional numerical solver such as FEM solves the outer region. Interestingly, BL-PINN is 480 capable of correctly resolving the boundary layer region as well as the interface, however, it struggles 481 to find the correct solution in the outer region where the original advection-diffusion equation is 482 solved without any special treatment. Finally, we demonstrated an example of inverse modeling 483 with BL-PINN (test case 5). More complicated inverse modeling examples such as finding velocity 484 fields from concentration (Raissi et al., 2020) could be investigated for boundary layers in future 485 work. 486

#### 487 5. Conclusion and Future Directions

We presented BL-PINN, a new theory-guided/model-driven extension of PINN for solving thin 488 boundary layer problems. In the benchmark problems investigated, BL-PINN demonstrated ex-489 cellent results and significantly outperformed prior PINN approaches, which could not provide 490 any meaningful results for solutions containing large gradients. BL-PINN was designed based on 491 asymptotic expansions and singular perturbation theory, and therefore the designed network is par-492 tially interpretable. Finally, thanks to the analytical incorporation of the perturbation parameter 493 in asymptotic expansions, BL-PINN naturally incorporates the perturbation parameter of interest 494 (e.g., diffusion coefficient) and does not need to be retrained during parametric evaluations. 495

There are several additional problems for which BL-PINN could potentially be utilized. Deep-496 ONets (Lu et al., 2021) and physics-informed DeepONets (Wang et al., 2021b) have been recently 497 introduced for learning operators and parametric solutions. Theory-guided and model-driven de-498 signs similar to BL-PINN could be used to facilitate parametric learning of problems where variation 499 in parameters leads to extreme behavior in the solution and large gradients. Boundary layer control 500 is another application area where flow measurement and data-driven modeling within boundary 501 layers are necessary (Bagheri et al., 2009; Belson et al., 2013). Unsteady boundary layers could 502 occur for systems of differential equations with multiscale temporal behavior, where the solution 503 rapidly changes in time (Verhulst, 2005; Kutz, 2020). BL-PINN could be applied to such dynam-504 ical systems problems. Characterizing multiple time-scale behavior in chaotic dynamical systems 505 with perturbation methods is another relevant example (Mease et al., 2016). Singular perturbation 506 problems also occur in systems of reaction-diffusion or advection-diffusion-reaction equations that 507 are commonly used in modeling the spatiotemporal dynamics of disease (Panfilov et al., 2019). 508 Finally, similar singular perturbation methods could be used in modeling low Reynolds number 509 hydrodynamics (Masoud and Stone, 2019). 510

#### 511 Conflict of Interest

512 The authors declare no conflict of interest.

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#### 516 Data Availability

The Pytorch codes and data used to generate the results in the manuscript are available on https://github.com/amir-cardiolab/BL-PINN/

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#### **Declaration of interests**

☑ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

□ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

## **Author Statement**

**Amirhosseion Arzani**: Conceptualization, Methodology, Software, Writing - Original Draft, Writing - Review & Editing, Funding acquisition. **Kevin Cassel**: Methodology, Writing - Review & Editing, **Roshan D'Souza**: Writing - Review & Editing, Funding acquisition.