PHYSICS-INFORMED NEURAL NETWORKS FOR SIMULATING 1D AND 2D HEAT TRANSFER EQUATIONS

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FINAL YEAR DESIGN PROJECT REPORT

This Report Presented in Partial Fulfillment of the Requirements for the Degree of Bachelor of Science in Computer Science and Engineering

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APPROVAL

This Project titled **"Physics-Informed Neural Networks for Simulating 1D and 2D Heat Transfer Equations"**, submitted by **Tamanna Tahmin** to the Department of Computer Science and Engineering, Daffodil International University, has been accepted as satisfactory for the partial fulfillment of the requirements for the degree of B.Sc. in Computer Science and Engineering and approved as to its style and contents. The presentation has been held on **14th July, 2024.**

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DECLARATION

We hereby declare that this project has been done by us under the supervision of **Ms. Shayla Sharmin, Senior Lecturer, Department of Computer Science and Engineering, Daffodil International University**. We also declare that neither this project nor any part of this project has been submitted elsewhere for the award of any degree or diploma.

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Abstract

In this study, we present the simulation of 1D and 2D heat transfer equations using physics-informed neural networks (PINNs) to predict temperature distributions over time. PINNs leverage the underlying physical laws governing heat diffusion, integrating these principles directly into the neural network training process. This approach ensures accurate, physically consistent simulations even with limited data. We applied PINNs to solve the heat equation in both one-dimensional and two-dimensional domains, demonstrating their efficacy in capturing the temporal evolution of temperature profiles. The simulations were conducted for various time intervals, highlighting the model's ability to generalize across different temporal scales. PINNs offers a simpler and more efficient computational process compared to traditional numerical and analytical methods, particularly for higher-dimensional equations. This work underscores the potential of PINNs to solve complex physics-based problems with greater efficiency and less complexity, highlighting their promise as powerful tools in engineering and scientific applications.

Keywords: PINNs, Simulations, Forward Problem, 1D and 2D heat equations

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Chapter 1

Introduction

1.1 Introduction

The application of machine learning (ML) in addressing heat transfer issues began in the 1990s with the introduction of artificial neural networks (ANN) to learn convective heat transfer coefficients from data [1]. Recently, advancements in learning-based techniques, supported by enhanced hardware like GPU technology, have significantly contributed to solving diverse heat transfer challenges [2-4]. Convolutional neural networks (CNNs), a popular deep learning technique, have been effectively used to make predictions from image-like data in complex, high-dimensional problems. For instance, a CNN was utilized to predict the local heat flux in turbulent channel flows using wall-shear stress and wall pressure as inputs [5]. Another example involves a CNN based on the U-net architecture, which used a 2D slice of the time-averaged temperature field to predict a ridge pattern for quantifying turbulent heat transfer variability [6]. These methods typically employ supervised learning, requiring labeled data (ground-truth) for training. Although these data-driven approaches offer rapid prediction once trained, generating the necessary data is challenging, and the models may not generalize well to different experimental conditions.

Beyond supervised learning, unsupervised learning has been explored, such as in a conjugate thermal optimization problem [7]. Recently, deep reinforcement learning (RL) has been applied to thermal system control. For example, RL-based control demonstrated the ability to stabilize the conductive regime and delay the onset of convection to a higher Rayleigh number, surpassing traditional linear controllers [8]. RL has also been applied to various convection problems [9], showing that it can enhance heat transfer performance by mitigating convection onset issues.

However, these efforts often overlook the underlying physics of heat transfer problems. To address this, multitask learning approaches like physics-informed neural networks (PINNs) have been introduced [10]. Initially proposed to solve forward and inverse problems combining data and partial differential equations (PDEs) [11], PINNs have been applied to numerous fluid mechanics and heat transfer problems [12]. For example, to understand the mechanisms of heat transfer enhancement in rough turbulent Rayleigh–Bénard convection, researchers used PINNs to predict turbulent transport in a specific subdomain filled with water and containing roughness elements on the hot plate, benefiting from extensive direct numerical simulations [13]. Additionally, NVIDIA's SimNet, based on PINNs, has been used to tackle multiphysics problems, including heat transfer in FPGA heat sinks within channels [14].

Moreover, from a mathematical perspective, manufacturing processes involving multiple transformations (e.g., phase changes in additive manufacturing or convective curing of composites) are governed by PDEs based on conservation laws of mass, momentum, and energy [15, 16]. Controlling the material behavior during these processes is crucial for ensuring quality, often achieved by precisely managing boundary conditions like pressure and temperature. These processes are typically studied using numerical methods such as finite elements (FE) and validated with in-process measurements from sensors [17]. However, the complexity of these processes, along with variable boundary conditions and the challenge of accurately measuring material behavior, makes control difficult. For instance, in convective heating, airflow variations can create thermal gradients and lags, complicating the control of part temperatures in ovens [18].

Following established approaches for solving PDEs using machine learning [19-21], this study develops a PINN to solve the heat transfer PDE in 1D and 2D scenarios within a representative manufacturing context. Physics-informed features based on heat transfer theory are engineered to accurately capture the underlying physics with the trained PINN. This method allows PINNs to predict heat transfer beyond their training zones, enabling rapid evaluation of heat transfer problems with different BCs. In an Industry 4.0 setting, this facilitates the development of near real-time feedback control loops to adjust process parameters and manage the part's temperature history.

1.2 Motivation

The primary motivation behind this research lies in the need to enhance the accuracy, efficiency, and applicability of modeling heat transfer phenomena, which are critical in various scientific and engineering domains. Traditional numerical methods for solving heat transfer equations often face limitations in terms of computational cost, scalability, and handling complex boundary conditions. By leveraging physics-informed neural networks (PINNs) with the PyTorch library, this research aims to overcome these challenges and offer a more robust and versatile approach.

Heat transfer is a fundamental aspect in numerous applications, from industrial processes and renewable energy systems to climate modeling and biomedical engineering. Accurate simulations of heat transfer are crucial for optimizing the design and operation of systems in these fields, leading to improved efficiency, safety, and performance. PINNs provide a powerful tool to achieve this by integrating the governing physical laws directly into the neural network training process, ensuring that the solutions adhere to the underlying physics.

Moreover, the use of the PyTorch library allows for leveraging advanced deep learning techniques, enabling efficient handling of large datasets and complex simulations. This research is motivated by the potential to significantly advance the state-of-the-art in thermal modeling, providing a more flexible and scalable solution that can be applied to a wide range of real-world problems. The ultimate goal is to contribute to scientific advancement and technological innovation by offering a superior method for solving and simulating heat transfer equations, thereby addressing critical challenges in various industries and promoting sustainable development.

1.3 Rationale of This Study

The rationale behind this study is diverse and aims to address several key limitations and opportunities in the field of heat transfer modeling through the application of physics-informed neural networks (PINNs). The study's rationale can be summarized in the following points:

1. **Limitations of Traditional Methods**:
    - **Computational Cost**: Traditional numerical methods like finite element and finite difference methods often require significant computational resources, especially for high-dimensional problems.
    - **Scalability Issues**: These methods struggle to scale efficiently, making it difficult to handle large and complex simulations effectively.
    - **Complex Boundary Conditions**: Traditional methods have limitations in managing intricate boundary conditions and heterogeneous material properties, which are common in real-world scenarios.
2. **Advantages of PINNs**:

- **Integration of Physical Laws**: PINNs incorporate the governing physical laws directly into the neural network training process, ensuring that the solutions are physically consistent and accurate.
- **Reduced Computational Burden**: By leveraging neural networks, PINNs can significantly reduce the computational cost compared to traditional methods, making them more suitable for large-scale and real-time applications.
- **Flexibility and Generalization**: PINNs are highly flexible and can generalize well to different scenarios and boundary conditions, enhancing their applicability across various domains.

3. **Utilization of Advanced Deep Learning Tools**:
   - **PyTorch Library**: Using the PyTorch library allows for leveraging advanced deep learning techniques and efficient handling of large datasets and complex simulations.
   - **State-of-the-Art Frameworks**: PyTorch provides robust frameworks for implementing and optimizing neural networks, facilitating the development of high-performance PINNs.
4. **Application Potential**:
   - **Industrial Manufacturing**: Accurate thermal simulations can optimize processes such as welding, metal forming, and material synthesis, leading to improved product quality and reduced energy consumption.
   - **Renewable Energy Systems**: Enhanced thermal management in solar panels and wind turbines can increase efficiency and lifespan, supporting the transition to sustainable energy sources.
   - **Climate Science**: Improved climate models can lead to better predictions and mitigation strategies for climate change impacts, contributing to environmental conservation efforts.
   - **Biomedical Engineering**: Precise heat transfer models are crucial for the design and optimization of medical devices and treatments, improving patient outcomes and safety.
5. **Scientific and Technological Advancement**:

- **Innovation in Thermal Modeling**: This research aims to push the boundaries of current thermal simulation methodologies, providing a more effective tool for researchers and engineers.
- **Sustainable Development**: The outcomes of this study can lead to technological innovations that support sustainable development, reducing energy consumption and promoting environmentally friendly practices.

By addressing these points, the study aims to demonstrate the significant potential of PINNs in solving and simulating heat transfer equations more efficiently and accurately, ultimately contributing to advancements in various scientific and engineering fields.

1.4 Research Questions

1. How can physics-informed neural networks (PINNs) improve the accuracy of solving 1D and 2D heat transfer equations compared to traditional numerical methods?

- PINNs integrate the governing physical laws directly into the neural network training process, ensuring that the solutions adhere to the underlying physics. This direct incorporation reduces the approximation errors that can arise in traditional numerical methods, leading to more accurate solutions. Additionally, PINNs are able to handle complex boundary conditions and heterogeneous material properties more effectively.

2. What are the computational advantages of using PINNs for heat transfer simulations?

- PINNs reduce the computational cost by leveraging the parallel processing capabilities of neural networks. Unlike traditional methods that may require extensive meshing and iterative solvers, PINNs can solve complex heat transfer problems with fewer computational resources. This efficiency is further enhanced by using advanced deep learning tools like the PyTorch library, which optimizes neural network performance.

3. In what ways can PINNs enhance the scalability of thermal simulations?

- PINNs are inherently scalable due to their neural network architecture, which can handle large datasets and complex simulations without a significant increase in computational time. This scalability allows PINNs to be applied to higher-dimensional problems and larger domains, which are challenging for traditional numerical methods.

4. How can the application of PINNs in thermal modeling contribute to industrial and technological advancements?

- By providing more accurate and efficient thermal simulations, PINNs can optimize industrial processes such as welding, metal forming, and material synthesis. This optimization leads to improved product quality, reduced material waste, and lower energy consumption. In renewable energy systems, enhanced thermal management can increase the efficiency and lifespan of solar panels and wind turbines. These advancements contribute to economic growth and support the transition to sustainable energy sources.

5. What potential does this research have in improving climate models and environmental monitoring?

- PINNs can enhance the accuracy of climate models by providing precise simulations of heat transfer in natural ecosystems. This improved accuracy can inform better predictions and mitigation strategies for climate change impacts. In environmental monitoring, PINNs can model the thermal effects of pollutants, enabling timely interventions to protect ecosystems and biodiversity.

6. How does this research prepare future engineers and scientists for applying advanced thermal simulation techniques?

Integrating the outcomes of this research into educational programs equips students with practical insights and hands-on experience in using PINNs for thermal simulations. This preparation ensures that future professionals are adept at applying cutting-edge technologies to solve complex problems, advancing the field of thermal engineering and promoting innovative solutions.

7. What are the ethical considerations associated with the application of PINNs in solving heat transfer problems?

- Ethical considerations include ensuring transparency in the development and deployment of PINNs, protecting data privacy and security, addressing biases in the models, and minimizing the environmental impact of computational resources. Researchers must also establish guidelines to prevent the misuse of PINNs for harmful purposes and consider the long-term societal impacts, such as potential changes in job markets and workforce displacement.

1.5 Expected Output

1. Enhanced Accuracy in Heat Transfer Simulations:

- **High-Fidelity Models**: Development of PINNs that provide more accurate solutions to 1D and 2D heat transfer equations with less physics and data-based loss.
- **Validation Results**: Demonstration of the models' accuracy through validation against known analytical outcomes and benchmark problems.

2. Reduced Computational Costs:

- **Efficiency Metrics**: Quantitative analysis showing reduced computational resources and time required by PINNs compared to traditional methods.
- **Scalability Demonstration**: Evidence that PINNs can efficiently handle larger and more complex simulations without a significant increase in computational cost.

3. Practical Applications:

- **Industrial Process Optimization**: Case studies or examples where PINNs are applied to optimize thermal processes in industries such as manufacturing, leading to improved product quality and reduced energy consumption.
- **Renewable Energy Systems**: Demonstrations of enhanced thermal management in renewable energy systems, such as solar panels and wind turbines, resulting in increased efficiency and lifespan.
-

4. Advanced Educational Tools:

- **Teaching Modules**: Development of educational materials and teaching modules that incorporate PINNs for thermal simulations, preparing students to use these advanced techniques in their careers.
- **Training Workshops**: Conducting workshops or seminars to train engineers and scientists on the practical applications of PINNs in solving heat transfer problems.

5. Framework and Algorithms:

- **Open-Source Code**: Release of the developed PINNs models and algorithms as open-source code, enabling other researchers and practitioners to replicate and build upon the work.
- **Documentation and Guidelines**: Comprehensive documentation and guidelines for implementing and applying PINNs to various heat transfer problems.

6. Environmental and Sustainability Impact:

- **Case Studies**: Examples of how PINNs can be used to model and mitigate the thermal effects of pollutants in natural ecosystems, supporting environmental conservation efforts.
- **Energy Efficiency Improvements**: Documentation of improvements in energy efficiency in industrial applications and renewable energy systems achieved through the application of PINNs.

7. Ethical and Responsible AI Use:

- **Ethical Guidelines**: Establishment of ethical guidelines for the development and deployment of PINNs, ensuring transparency, fairness, and data privacy.
- **Impact Assessments**: Regular assessments of the societal and environmental impacts of the research outcomes, ensuring long-term positive contributions.

1.6 Report Layout

This report is organized into six distinct chapters, each contributing uniquely to the overall narrative. Chapter 1, titled "Introduction," sets the stage by providing a comprehensive overview of the project's inception, articulating its objectives, motivations, and anticipated outcomes. This initial chapter also delivers a detailed project description, laying the groundwork for the discussions that follow.

Chapter 2, "Background" offers an in-depth analysis of existing literature relevant to the project. This thorough exploration establishes a solid contextual foundation and situates the project within the broader field.

In Chapter 3, "Methodology" the focus transitions to the procedural elements of the project. This chapter meticulously outlines the research methods employed, highlighting their significance in shaping the project's design and execution.

Chapter 4, "Results and Discussions" is dedicated to presenting and examining the findings of the project. This chapter provides a detailed analysis and interpretation of the results, offering critical insights and conclusions drawn from the data collected.

Chapter 5, “Social and Environment impacts” addresses the constraints and challenges encountered during the project's execution. This chapter enhances transparency by explicitly discussing the limitations, thereby providing a balanced view of the project's scope and reliability.

The final chapter, Chapter 6, "Conclusion and Future Scope," encapsulates the project's main findings and provides a succinct summary. This chapter also proposes potential directions for future research and development, concluding the report with forward-looking insights.

The structured approach of the report ensures a logical progression of information, facilitating a comprehensive and coherent narrative from the project's inception to its conclusion. This systematic organization not only aids in the clear presentation of the project's various facets but also enhances the overall understanding and impact of the research.

Chapter 2

Background

2.1 Previous works

Physics-Informed Neural Networks (PINNs) have emerged as a transformative approach in heat transfer research, bridging the gap between physics-based modeling and data-driven techniques. Initially proposed by Raissi et al. [11], PINNs integrate physical laws directly into neural networks, enabling the solution of partial differential equations (PDEs) governing heat transfer phenomena with high accuracy and computational efficiency. This foundational work demonstrated PINNs' superiority over traditional numerical methods in capturing complex spatial and temporal variations in temperature distributions. Subsequent studies have expanded the application scope of PINNs across diverse heat transfer problems. For instance, Zhang et al. applied PINNs to transient heat conduction in heterogeneous media, highlighting their ability to model dynamic thermal behaviors and material heterogeneity effectively [22]. Son et al. utilized PINNs for optimizing thermal management systems in electronic cooling devices, showcasing their role in improving system efficiency through accurate temperature prediction and design optimization [23]. Moreover, PINNs have been integrated with finite element methods (FEM) to tackle multi-dimensional heat transfer problems with complex geometries and boundary conditions, demonstrating enhanced computational efficiency and scalability. Zhang et al. further extended this approach to transient heat transfer problems in industrial applications, emphasizing capability of PINNs to model real-time thermal responses in complex engineering systems [24].

The versatility of PINNs extends beyond traditional heat conduction problems. Brycov et al. explored their application in modeling heat transfer in porous media, illustrating how PINNs can handle the intricate flow and thermal interactions within porous structures [25]. Yang et al. enhanced PINNs capabilities by integrating them with long short-term memory networks, enabling robust modeling of time-dependent heat transfer processes [26]. Lu et al. introduced interpretable and stable deep learning techniques within the context of multiscale heat transfer, advancing the understanding and predictability of complex thermal phenomena [27]. Additionally, Koric et al. utilized PINNs for data-driven discovery of optimal heat transfer surfaces, demonstrating their potential in optimizing heat exchange efficiency through innovative design approaches [28].

The integration of PINNs with experimental data and validation techniques has further bolstered their applicability in real-world scenarios, ensuring robustness and reliability in predictions. This interdisciplinary approach has not only advanced fundamental understanding but also opened new avenues for addressing challenges such as uncertainty quantification and multi-physics coupling in heat transfer research.

Overall, the evolution of PINNs represents a paradigm shift in computational heat transfer modeling, offering unparalleled capabilities in leveraging data-driven insights while respecting physical principles. As ongoing research continues to refine methodologies and expand application domains, PINNs are poised to play a pivotal role in shaping the future of thermal sciences and engineering design.

2.2 Scope of this Study

The scope of my research involved utilizing PINNs to solve one-dimensional (1D) and two-dimensional (2D) heat transfer equations. The research gap addressed by this study lies in the limitations and challenges associated with traditional numerical methods for solving heat transfer problems, such as finite element, finite difference, and finite volume methods.

Traditional numerical methods often require extensive computational resources and can become inefficient or unstable, especially when dealing with complex geometries, boundary conditions, or highly non-linear problems. Moreover, these methods may not seamlessly integrate with data-driven approaches, which are increasingly important in modern scientific and engineering problems.

PINNs offer a novel approach by leveraging the strengths of both machine learning and classical physics. They use neural networks to approximate the solution of partial differential equations (PDEs), incorporating the physical laws governing the system directly into the training process. This method can potentially reduce computational costs, improve scalability, and provide more accurate solutions even with limited data.

The research gap thus encompasses:

1. **Efficiency and Computational Cost:** Traditional methods can be computationally intensive. PINNs have the potential to solve PDEs more efficiently, making them suitable for real-time applications and large-scale problems.

2. **Integration with Data:** PINNs can naturally integrate experimental or observed data into the solution process, which is a significant advantage over conventional methods that typically rely solely on initial and boundary conditions.

3. **Flexibility and Generalization:** PINNs are flexible in handling complex geometries and boundary conditions, and they can generalize well across different scenarios without significant modifications to the underlying method.
4. **Non-linearity and Complexity:** Many real-world heat transfer problems involve non-linear and complex interactions that are challenging for traditional methods. PINNs can handle these complexities more effectively.

By addressing these gaps, my research aims to demonstrate the efficacy of PINNs in solving 1D and 2D heat transfer equations, providing a viable alternative to traditional numerical methods and advancing the field of computational heat transfer.

2.3 Challenges

During the research on solving 1D and 2D heat transfer equations using Physics-Informed Neural Networks (PINNs), several challenges were encountered that needed to be addressed effectively:

1. **Loss Function Design**: One of the primary challenges was designing an effective loss function for the PINNs. The loss function needed to balance the fidelity to the governing heat transfer equations (ensuring physical consistency) with the ability to generalize and learn from the available data. Finding the right formulation that captures both aspects accurately was crucial for achieving reliable and accurate results.
2. **Training Instability**: Neural networks, including those used in PINNs, can suffer from training instability, particularly when dealing with PDEs with complex geometries or highly non-linear behavior. Techniques such as adaptive learning rates, regularization, and careful initialization of network parameters were employed to mitigate instability and improve convergence.
3. **Data Scarcity and Quality**: Obtaining sufficient and high-quality data for training the PINNs posed another challenge. In many cases, data for boundary conditions or initial conditions might be limited or noisy. Techniques such as data augmentation, synthetic data generation, and careful preprocessing were necessary to ensure robust training and generalization of the models.

4. **Dimensionality and Computational Resources**: Handling 2D heat transfer problems introduced significant computational challenges compared to 1D problems. The increased dimensionality requires more computational resources and careful optimization of network architectures and training procedures to maintain efficiency without sacrificing accuracy.
5. **Model Interpretability**: Neural networks are often considered black-box models, making it challenging to interpret how they arrive at their predictions. For scientific applications like heat transfer, understanding the underlying physical principles learned by the network and ensuring the results align with known physics was crucial. Techniques such as sensitivity analysis and model explainability methods were explored to enhance interpretability.
6. **Integration with Existing Tools**: Integrating PINNs into existing workflows and tools used in computational heat transfer research required careful consideration. Compatibility with traditional numerical methods, validation against benchmark problems, and comparison with analytical solutions were essential steps to validate the efficacy and reliability of PINNs in this domain.

Chapter 3

Research Methodology

3.1 Physics-Informed Neural Networks

A machine learning technique known as the Physics-Informed Neural Network (PINN) can be employed to approximately solve partial differential equations (PDEs). The general form of PDEs, along with their initial and boundary conditions, is:

$$u_t + \mathcal{N}_x[u] = 0, \quad x \in \Omega, t \in [0, 1]$$

$$u(x, 0) = h(x), \quad x \in \Omega \qquad (1)$$

$$u(x, t) = g(x, t), \quad x \in \partial\Omega, t \in [0, T]$$

Let $\mathcal{N}_x$ represent a general linear or nonlinear differential operator. Here, $x \in \mathbb{R}^d$ and t correspond to the spatial and temporal coordinates, respectively. Ω and $\partial\Omega$ refer to the computational domain and its boundary. The function u(x, t) is the solution to the PDEs, subject to the initial condition h(x) and the boundary condition g(x, t). It is important to note that this formulation can be extended to higher-order PDEs because they can be transformed into systems of first-order PDEs.

A PINNs model consists of two primary sub-networks: an approximator network and a residual network [29]. When provided with the input (x, t) and trained, the approximator network generates an approximate solution, denoted as u(x, t) as mentioned above. The training process involves the use of a grid of points, known as collocation points, which are sampled either randomly or systematically from the simulation domain. The approximator network's trainable parameters, which include weights and biases, are optimized by minimizing a composite loss function structured according to the following equations (Eq. 2 & 3):

$$L = L_r + L_o + L_b \qquad (2)$$

$$L_r = \frac{1}{N_r}\sum_{i=1}^{N_r}\left|u(x^i, t^i) + N\left[u\left(x^i, t^i\right)\right]\right|^2$$

$$L_o = \frac{1}{N_o}\sum_{i=1}^{N_o}\left|u\left(x^i, t^i\right) - h^i\right|^2 \qquad (3)$$

$$L_b = \frac{1}{N_b}\sum_{i=1}^{N_b}\left|u\left(x^i, t^i\right) - g^i\right|^2$$

In this context, L_r, L_o, and L_b denote the residuals of the governing equations, initial conditions, and boundary conditions, respectively. Similarly, N_r, N_o, and N_b represent the number of collocation points for the computational domain, initial conditions, and boundary conditions, respectively. The residual network, which is a non-trainable component of the PINN model, is responsible for computing these residuals. To compute the residual L_r, PINNs require the derivatives of the outputs with respect to the inputs x and t. This computation is carried out using automatic differentiation, which leverages the chain rule to combine the derivatives of the constituent operations to obtain the derivative of the entire function. This method is essential for the development of PINNs and distinguishes them from earlier methods in the 1990s that depended on manually derived back-propagation rules. Currently, automatic differentiation is a well-established feature in most deep learning frameworks, including TensorFlow and PyTorch, which eliminates the need for tedious manual derivations or numerical discretization and allows for the computation of derivatives of all orders in space and time.

Figure 1 illustrates the schematic of the PINNs framework, utilizing a basic heat equation "$u_t = \alpha\, u_{xx}$" as an illustrative example for setting up PINNs in heat transfer applications. In Fig. 1(a), a fully connected neural network approximates the solution u(x, t) contributing to the construction of the residual loss L_r, boundary conditions loss L_b and initial conditions loss L_o. The parameters of this network are optimized through gradient-descent methods via backpropagation of the loss function. Figure 1(b) depicts the distribution of data points used for different components of the loss function. It is important to note that the residual points for computing L_r can be randomly selected within the space-time domain, with the number of points determined by user-defined parameters.

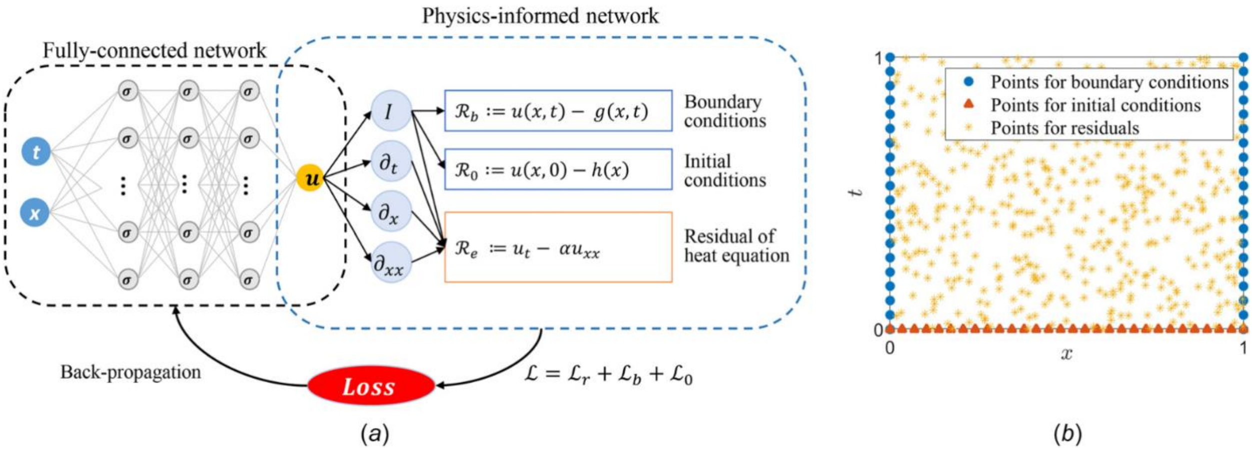

Figure 3.1.1: Overview of Physics informed Neural Networks (PINNs) [30]: (a) Schematic representation of PINNs framework (b) Illustration of point selection for PINNs in computational domain

3.2 Heat Transfer Equations

The heat transfer equation for a specific component can be expressed as follows [30]:

$$\frac{\partial}{\partial t}(\rho C_P T) = \frac{\partial}{\partial x}\left(k_{xx}\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial x}\left(k_{yy}\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k_{zz}\frac{\partial T}{\partial z}\right) + \dot{Q} \tag{4}$$

Herein, T represent temperature, ρ represent part density, C_P, k, $\dot{Q}$ are specific heat capacity, thermal conductivity, and the rate of heat generation within the part, respectively. For simplicity, this method will be described in the context of one-dimensional (1D) and two-dimensional (2D) heat transfer. However, this approach can be readily extended to higher dimensions, which will be covered elsewhere. In the case of 1D heat transfer with no heat generation term, the general heat equation can be simplified as follows, respectively:

$$\frac{\partial T}{\partial t} - \alpha\frac{\partial^2 T}{\partial x^2} = 0,\ x \in (0, 1),\ t \in (0, t) \tag{5}$$

With initial condition:

$$T(x, 0) = \sin(\pi x),\ 0 < x < 1$$

And boundary condition:

$$T(0, t) = 0 = T(1, t),\ 0 \le t \le 1$$

And in case of 2D heat transfer with no heat generation term, the general heat equation can be simplified as follows

$$\frac{\partial T}{\partial t} - \alpha\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) = 0,\ x, y \in (0,1),\ t \in (0, t) \quad (6)$$

With initial condition:

$$T(x, y, 0) = \sin(\pi x) \times \sin(\pi y),\ 0 < x, y < 1$$

And boundary condition:

$$T(x, 0, t) = T(x, 1, t) = 0 = T(0, y, t) = T(1, y, t),\ 0 \leq t \leq 1$$

Where the thermal diffusivity (α) can be defined as:

$$\alpha = \frac{k}{\rho C_P} \quad (7)$$

3.3 Implementation of PINNs

To develop the PINN model for simulating 1D and 2D heat transfer equations within the given initial and boundary conditions, we utilized the PyTorch library [31]. Our PINN architecture employs two inputs, (x, t) with three layers comprising a maximum of 64 neurons, all employing the 'tanh' activation function. The collocation points are categorized into two subsets: a principal subset of 1000 points representing the general problem domain, and a smaller test subset of 200 points. The test subset specifically enforces boundary and initial conditions, which are consistent across all test cases.

The training of the PINN model involves two phases. In the first phase, we optimize the weights and biases using the Adam algorithm over the data points, with a learning rate set to 10^{-3}. Following this, in the second phase, the Limited Memory Broyden–Fletcher–Goldfarb–Shanno (L-BFGS) algorithm refines the solution further, post a "global" search as described in [32] .The entire training process completes in approximately 40 seconds using a GeForce GTX 1660Ti GPU accelerator.

Exploring different hyper-parameters such as activation functions, training methodologies, and varying PINN architectures could potentially enhance performance. However, due to the exhaustive nature and beyond the scope of this study, we selected hyper-parameter values commonly found in the literature on heat transfer problems.

The primary objective of this study is to evaluate the applicability of PINNs model in solving and simulating two test problems of heat transfer equations in the given boundary conditions.

Chapter 4

Result and Discussion

4.1 1D Heat Equation

In the context of the one-dimensional (1D) heat transfer equation (Eq. 5), the thermal diffusivity coefficient (α) was assumed to be 1 W/m·K for all conditions. A 1-meter rod-like material was considered, with an initial condition represented by a sine wave propagating along its length, approximating the analytical solution of the equation. For the boundary conditions, both ends of the rod ($x = 0$ and $x = 1$) were maintained at zero temperature for all time values (t), while the midpoint was set to a maximum temperature of ~ 1. Consequently, it is anticipated that heat will transfer from the midpoint towards the ends, consistent with the principle that heat flows from regions of higher temperature to regions of lower temperature.

Upon solving the equation using PINNs, the results indicated that the temperature was highest (1) at the midpoint of the rod and zero at both ends (Fig.2 (a)). After 0.25 seconds, the heat had diffused towards the lower temperature regions, with the temperature distribution decreasing to a range of 0.01-0.09, which is ten times lower than the initial values (Fig.2 (b)). After 0.50 seconds, the temperatures further decreased significantly to a range of 0.001-0.009, which is one hundred times lower than the initial temporal distribution (Fig.2 (c)). This behavior is in accordance with the second law of thermodynamics, thereby validating our model.

For a clearer visualization of the temporal distribution, a single data slice was extracted at $t = 0$, 0.25, and 0.50, which clearly supports the contour map results shown in Figure 3. To further assess the accuracy of our model, the loss history of the training and test sets was recorded and plotted in Figure 4, in accordance with Equations 2 and 3. The results demonstrated that the loss for both the training and test sets was significantly reduced, approaching nearly zero values (6.72E-5 and 6.57E-5, respectively, as shown in Table 1). This confirms the high accuracy of the predictions made by the PINNs model.

This study exemplifies the robustness of using PINNs for solving heat transfer problems, showcasing their potential in accurately predicting temperature distributions over time. The adherence to the second law of thermodynamics further strengthens the validity of the model, highlighting its applicability in practical scenarios where precise thermal management is crucial.

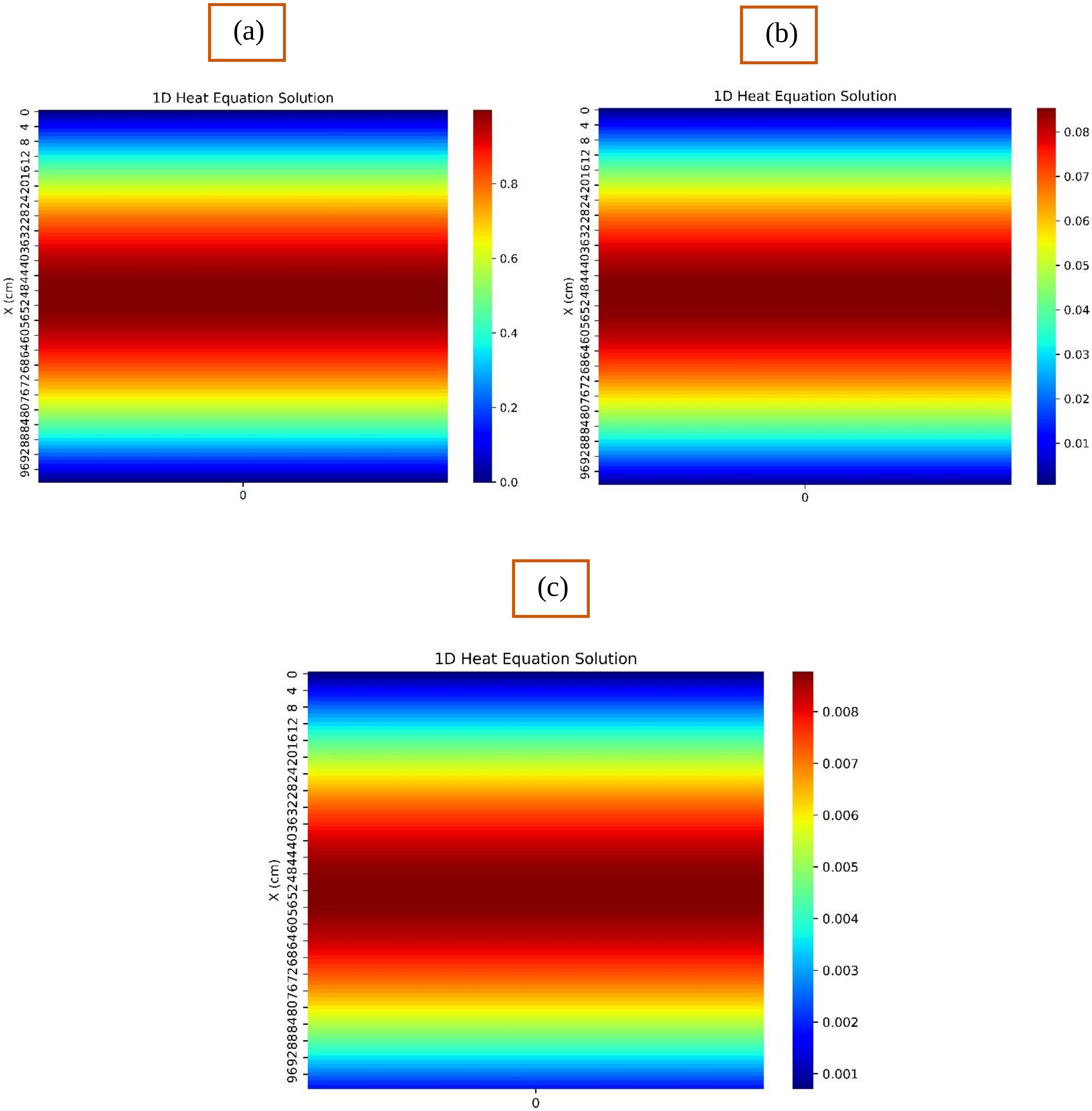

Figure 4.1.1: Temperature Distribution of 1D heat equation (a) 0 sec (b) 0.25 sec (c) 0.5 sec

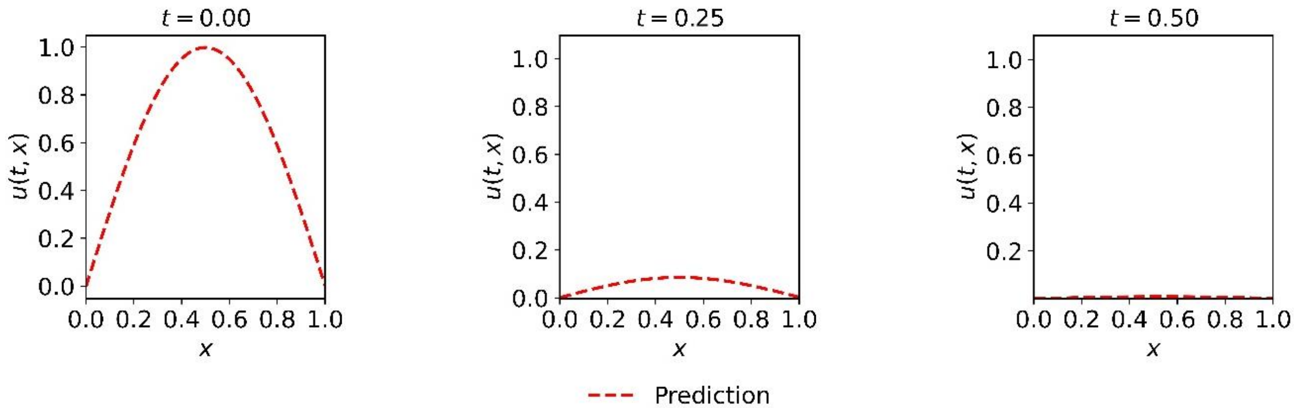

Figure 4.1.2: Single wave visualization of 1D heat equation at different time

Figure 4.1.3: Loss History of Training and Test set of 1D Equation

4.2 2D Heat Equation

Similarly, in 2D heat equation, the thermal diffusivity coefficient (α) was uniformly set to 1 W/m·K for all conditions in both the x and y directions. A 1-meter square material was examined, with its initial condition modeled by a sine wave propagating along its length, closely approximating the analytical solution of the equation. For the boundary conditions, the edges of the material (x, y = 0 and x, y = 1) were maintained at zero temperature for all time values (t), while the midpoint was set to a maximum temperature of approximately 1. This setup anticipates heat transfer from the midpoint towards the edges, adhering to the principle that heat flows from regions of higher temperature to regions of lower temperature.

Upon solving the equation using PINNs, the results showed that the temperature was highest (1) at the center of the square and zero at both edges (Fig. 5(a)). After 0.25 seconds, heat had diffused towards the lower temperature regions, with the temperature distribution decreasing to a range of 0.00-0.025, thirty times lower than the initial values (Fig. 5(b)). After 0.50 seconds, the temperatures further decreased significantly to a range of -0.006 to 0.002, two hundred times lower than the initial temporal distribution (Fig. 5(c)). This behavior aligns with the second law of thermodynamics, thus validating our model.

To further evaluate the accuracy of our model, the loss history of the training and test sets was documented and plotted in Figure 4, in accordance with Equations 2 and 3. The results demonstrated that the loss for both the training and test sets was significantly reduced, approaching nearly zero values (1.81E-3 and 2.43E-3, respectively, as shown in Table 1). This confirms the high accuracy of the predictions made by the PINNs model for higher dimensional equations.

Table 1: Final Loss for Train and Test Sets after Complete Iterations

Data	1D Equation	2D Equation
Train Set	6.72×10^{-5}	1.18×10^{-3}
Test Set	6.57×10^{-5}	2.43×10^{-3}

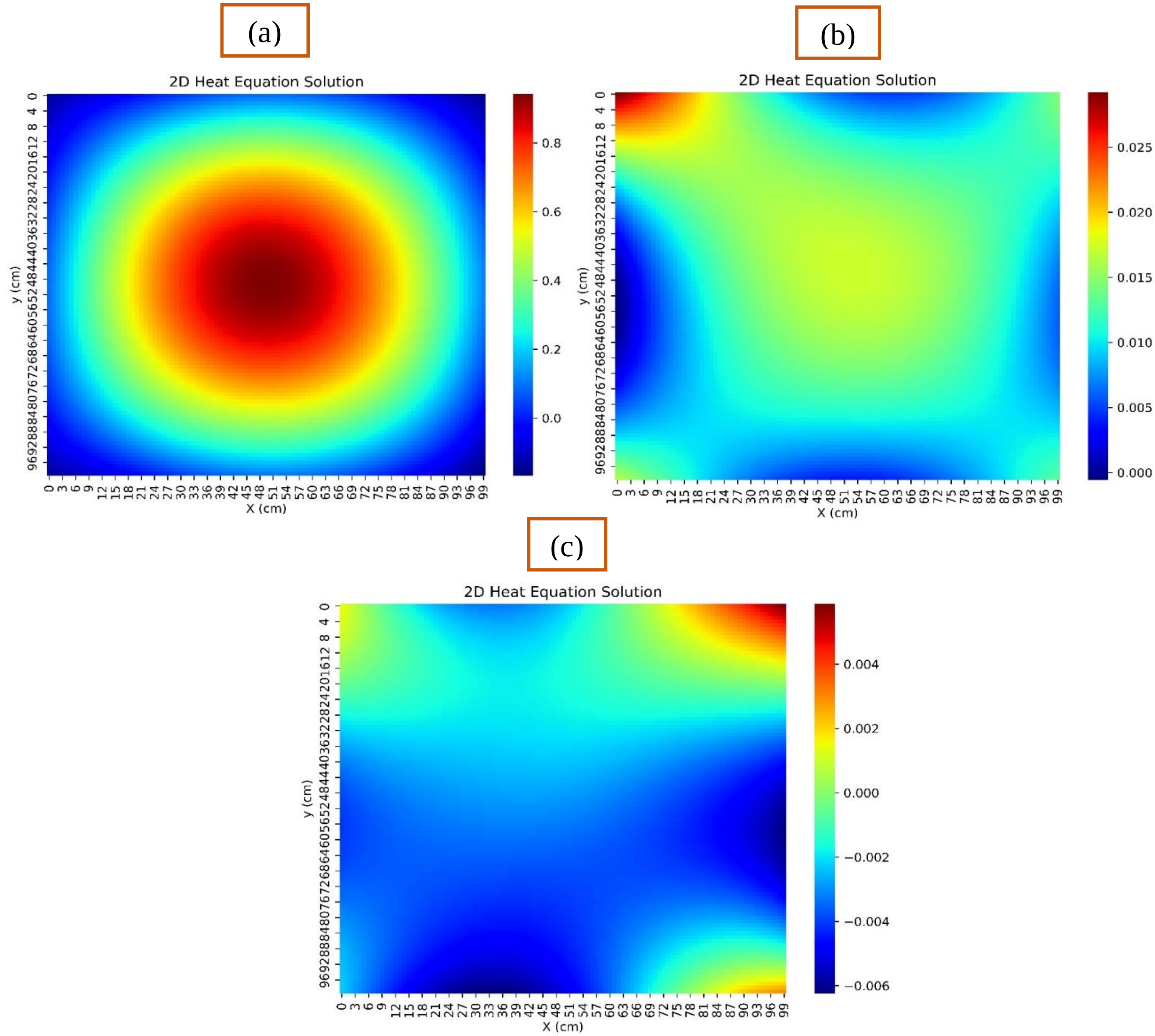

Figure 4.2.1: Temporal Distribution of 2D heat equation (a) 0 sec (b) 0.25 sec (c) 0.5 sec

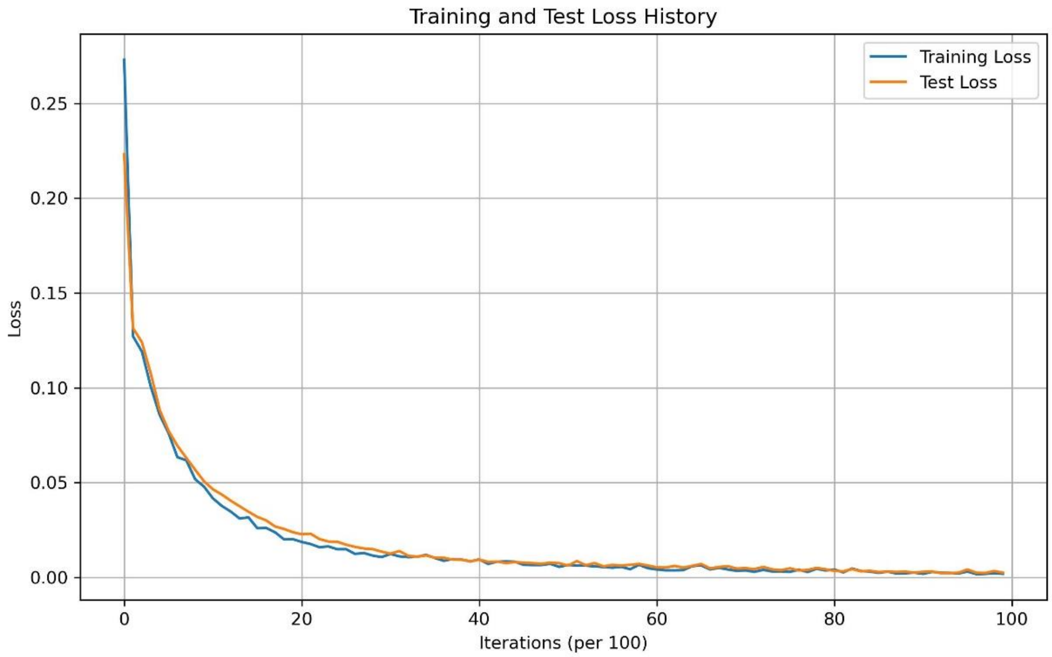

Figure 4.2.2: Loss History of Training and Test set of 1D Equation

Chapter 5

Impact on Society, Environment, Ethical Aspects and Sustainability

5.1 Impact on Society

The application of PINNs to solve and simulate 1D and 2D heat transfer equations has profound implications for society. By providing more accurate and efficient thermal simulations, this research can significantly enhance various sectors that depend on precise modeling of thermal processes.

In healthcare, improved simulations of heat transfer can aid in the design and optimization of medical devices, such as hyperthermia treatment equipment and cryotherapy devices. This leads to better patient outcomes, increased safety, and reduced healthcare costs. Additionally, accurate thermal models can improve the understanding of biological heat transfer, contributing to more effective treatments for thermal injuries and conditions.

The industrial sector, particularly in manufacturing, benefits from optimized thermal management solutions. This research can enhance the efficiency of processes such as welding, metal forming, and material synthesis. By improving the precision of these thermal processes, manufacturers can achieve higher product quality, reduce material waste, and lower energy consumption, leading to economic growth and competitiveness.

In education, the integration of advanced thermal simulations into engineering curricula can provide students with practical insights and hands-on experience. This prepares a new generation of engineers who are adept at using cutting-edge technologies to solve complex problems, thereby advancing the field of thermal engineering. Overall, this study drives innovation, enhances efficiency, and prepares society to better handle the challenges associated with thermal management across various fields.

5.2 Impact on Environment

Solving 1D and 2D heat transfer equations offers significant environmental benefits by enabling more accurate and efficient thermal simulations.

In renewable energy, PINNs can optimize the design and operation of solar panels and wind turbines by providing precise thermal management solutions. For instance, accurate simulations of heat distribution in photovoltaic cells can enhance their efficiency and lifespan, promoting the adoption of solar energy.

Similarly, optimizing thermal regulation in wind turbines can improve their performance and reduce maintenance needs, supporting the transition to cleaner energy sources.

In environmental monitoring, PINNs can be used to model heat transfer in natural ecosystems, such as the thermal effects of pollutants in water bodies. This enables timely interventions to prevent ecological damage and supports the preservation of biodiversity. Moreover, accurate thermal simulations can help in understanding and mitigating the impacts of urban heat islands, contributing to better urban planning and the creation of more sustainable cities.

PINNs can also aid in climate science by improving the accuracy of models that predict the effects of global warming. Enhanced thermal simulations can inform more effective climate policies and strategies for reducing greenhouse gas emissions, thereby helping to combat climate change.

Furthermore, the ability to efficiently model and manage heat transfer can reduce the energy consumption of industrial processes, leading to lower carbon footprints and less environmental pollution. This research thus supports the development of technologies and practices that are not only economically beneficial but also environmentally sustainable

5.3 Ethical Aspects

The ethical considerations of applying PINNs to solve heat transfer problems involve transparency, fairness, and responsibility. Ensuring transparency requires disclosing model assumptions and limitations to stakeholders, maintaining trust and accountability. Addressing bias is crucial, as PINNs, like all machine learning models, can perpetuate biases present in training data, potentially exacerbating societal inequalities. Protecting data privacy and security is essential, particularly with sensitive information used in simulations. Striving for environmental responsibility involves minimizing the carbon footprint of computational processes and promoting sustainable practices in applications. Additionally, ethical oversight is necessary to prevent misuse, such as unauthorized surveillance or discriminatory uses. By addressing these ethical dimensions, researchers can maximize the positive impacts of PINNs while mitigating potential risks and ensuring equitable and responsible deployment in various domains.

5.4 Sustainability Plans

The sustainability plans for utilizing the outcomes of this research are multi-faceted. Firstly, energy-efficient algorithms and renewable energy-powered data centers will be used to reduce the carbon footprint of computational processes. The optimized thermal management techniques developed will be applied to enhance the efficiency and longevity of renewable energy systems such as solar panels and wind turbines, promoting cleaner energy solutions. PINNs will also be used to model and mitigate thermal pollution in natural ecosystems, supporting proactive environmental conservation efforts. In industrial applications, the research will focus on reducing material waste and energy consumption, fostering sustainable manufacturing practices. Education and training programs will incorporate these advanced thermal simulation techniques, preparing future engineers and scientists to apply sustainable methods in their work. Collaborative efforts with industry stakeholders and policymakers will drive the adoption of these technologies in real-world settings, ensuring they contribute to sustainable development. Regular lifecycle assessments will ensure that the technologies meet sustainability standards, fostering continuous improvement and long-term positive environmental impacts.

Chapter 6

Conclusion

6.1 Conclusion

In this thesis, we successfully employed physics-informed neural networks (PINNs) using the PyTorch library to simulate 1D and 2D heat transfer equations, achieving highly accurate predictions of temperature distributions over time. Our approach demonstrated significant advantages over traditional numerical and analytical methods, particularly in terms of computational efficiency and simplicity. The final loss values for the training and test sets were remarkably low, with the 1D equation achieving losses of 6.72×10^{-5} and 6.57×10^{-5}, respectively, and the 2D equation achieving losses of 1.18×10^{-3} and 2.43×10^{-3}, respectively.

The implications of this work are substantial for scientific and industrial applications, especially within the context of Industry 4.0. PINNs offer a robust and efficient alternative to traditional methods, enabling the resolution of complex partial differential equations (PDEs) that are fundamental to numerous physical processes. Their ability to integrate physical laws directly into the learning process not only enhances accuracy but also reduces the computational burden typically associated with high-dimensional and complex systems.

This research highlights the potential of PINNs to revolutionize the way we approach problem-solving in various fields, including materials science, thermal engineering, and advanced manufacturing processes. By providing a more accessible and scalable solution for PDEs, PINNs can facilitate advancements in the design and optimization of industrial processes, leading to more efficient and cost-effective production methods. Moreover, the integration of PINNs into digital twins and predictive maintenance systems can significantly enhance the capabilities of smart manufacturing, aligning with the goals of Industry 4.0 to create intelligent and interconnected production environments.

In conclusion, this thesis demonstrates that physics-informed neural networks represent a promising tool for solving fundamental heat transfer problems and beyond. Their ability to streamline complex computations and improve predictive accuracy paves the way for further scientific advancements and practical applications across a wide range of disciplines.

6.2 Future Prospects

The findings of this thesis open several exciting avenues for future research and applications, particularly in addressing highly complex physics-based problems in real-world scenarios. Building on the demonstrated efficacy of physics-informed neural networks (PINNs) in solving 1D and 2D heat transfer equations, future work can extend this approach to tackle more intricate and higher-dimensional partial differential equations (PDEs) across different scientific and engineering domains. Moreover, in real cases, convection and radiation also takes place near the boundary of heat conduction. Therefore, combining convection and radiation in boundary conditions and solving the hybrid PDE with PINNs can successfully simulate the industrial scenario, which is very difficult to avail by other computational tools.

Furthermore, one significant area of potential is in climate modeling and environmental science. PINNs can be applied to simulate atmospheric dynamics, ocean circulation, and climate change impacts with greater accuracy and computational efficiency than traditional methods. This can enhance predictive capabilities for weather forecasting, natural disaster management, and environmental conservation efforts.

In biomedical engineering, PINNs offer promising applications in modeling biological processes and systems. For instance, they can be used to simulate blood flow dynamics in cardiovascular research, tissue growth and healing processes, and the spread of infectious diseases. These models can improve patient-specific treatment plans and contribute to the development of advanced medical devices.

The energy sector can also benefit greatly from the adoption of PINNs. In renewable energy, they can optimize the design and operation of solar panels, wind turbines, and energy storage systems by accurately modeling fluid dynamics, thermal processes, and material properties. This leads to more efficient energy production and storage solutions, which are critical for sustainable development.

Additionally, PINNs have substantial potential in the field of aerospace engineering. They can be employed to solve complex fluid dynamics problems, such as airflow over aircraft wings, thermal protection systems for re-entry vehicles, and the design of hypersonic vehicles. The improved accuracy and reduced computational cost of PINNs make them invaluable for optimizing performance and safety in aerospace applications.

In the realm of smart manufacturing and Industry 4.0, PINNs can be integrated into digital twin frameworks to create real-time, data-driven models of manufacturing processes. This enables predictive maintenance, process optimization, and fault detection, leading to enhanced efficiency, reduced downtime, and lower operational costs.

Moreover, future research can explore the integration of PINNs with machine learning techniques such as reinforcement learning and unsupervised learning to further improve their adaptability and performance in dynamic and uncertain environments. The development of hybrid models combining PINNs with traditional numerical methods could also enhance their robustness and applicability to a wider range of problems.

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Appendix A

Course Outcomes, Complex Engineering Problems (EP) and Complex Engineering Activities (EA) Addressing

Title:

PHYSICS-INFORMED NEURAL NETWORKS FOR SIMULATING 1D AND 2D HEAT TRANSFER EQUATIONS

Student ID: [Student ID]

CO Description for FYDP

CO	CO Descriptions	PO
Phase -I		
CO1	Integrate recently gained and previously acquired knowledge to implement **P I N N S M O D E L in Heat Transfer Problems** for the Final Year Design Project (FYDP)	**PO1**
CO2	Analyze different aspects of the goals in designing a solution for this FYDP	**PO2**
CO3	Explore diverse problem domains through a literature review, delineate the issues, and establish this goals for the FYDP	**PO4**
CO4	Perform economic evaluation and cost estimation and employ suitable project management procedures throughout the development life cycle of the FYDP	**PO11**
Phase -II		
CO5	Design and develop technical solutions and system components or processes that meet specified requirements, ensuring compliance with public health and safety standards, as well as considering cultural, socioeconomic, and environmental factors in this FYDP	**PO3**
CO6	Choose and apply appropriate methodologies, resources, and contemporary engineering and IT technologies to address complex engineering processes, encompassing prediction and modeling, while adhering to relevant constraints in this FYDP	**PO5**
CO7	Analyze societal, health, safety, legal, and cultural considerations, along with associated responsibilities, in the context of professional engineering practice and the resolution of this problem, employing logical reasoning guided by contextual understanding.	**PO6**
CO8	Comprehend and evaluate the enduring sustainability and impact of professional engineering endeavors in addressing intricate engineering challenges within social and environmental frameworks.	**PO7**

CO9	Implement ethical principles and adhere to professional standards and norms in this FYDP	**PO8**
CO10	Capable of operating proficiently both individually and as a team member or leader across diverse teams and interdisciplinary settings in this FYDP.	**PO9**

CO11	Proficiently communicate with the engineering community and broader society regarding complex engineering endeavors, including the ability to comprehend and generate comprehensive reports and design documentation, as well as provide and receive clear instructions throughout this FYDP.	**PO10**
CO12	Acknowledge the importance of self-directed and life-long learning within the evolving landscape of technology, and possess the readiness and capability to engage in lifelong learning endeavors.	**PO12**

Addressing CO (1 to 8), Knowledge Profile (K), Attainment of Complex Engineering Problems (EP), and Attainment of Complex Engineering Activities (EA)

Addressing CO (1 to 8), Knowledge Profile (K), Attainment of Complex Engineering Problems (EP):

SN	EP Definition	Attainment	CO	Justification (with Knowledge Profile)	References
1.	**EP1: Depth of Knowledge required**	Yes	CO1, CO2, CO3, CO5, CO6, CO7 and CO8	This project demonstrates **Physics-Informed Neural Network** model by employing deep neural networks, data augmentation techniques for derivative Heat Transfer equation. The project demonstrates **specialist knowledge (K4)** by conducting Deep learning with advanced model where Physics-based Partial Differential Equation incorporated in it.	**Page no:** [14-17] **Section:** [3.3] **Page no:** [16-18] **Section:** [3.1]
				The project applies **engineering practice & design (K5)** by the figure of process of experiments. The project addresses	**Page no:** [19-22]

				engineering practice & technology (K6) by employing PINNs model.	**Section:** [4.0] [14-19]
					Section: [4.0]
				This project ensures to **K8 (Research Literature)** by synthesizing insights from recent studies, to advance medical herbs detection using deep learning, showcasing a comprehensive understanding of current methodologies.	**Page no:** [10-12] **Section:** [2.2]
2.	**EP2: Range of Conflicting Requirements**	Yes	CO2, and CO7	This project addresses **EP-2** by solving Heat transfer equations, addressing limitations of traditional methods and the complexities of integrating deep learning. Through comparative analysis, it confronts challenges in understanding spatial distributions, offering insights for refining conventional methodologies.	**Page no:** [3, 11-12] **Section:** [1.3,2.3]
3.	**EP3: Depth of analysis required**	Yes	CO2, and CO6	This project addresses **EP-3** by meticulously comparing experimental outcomes, highlighting Deep Learning as the chosen significant solution for 1D and 2D Heat Transfer Equations.	**Page no:** [19-22] **Section:** [4.0]

4.	**EP4: Familiarity of Issues**	Yes	CO8	This project's interdisciplinary approach extends beyond computer science and engineering, impacting Heat Transfer scenarios, contributing to advancements in public Industrial Process and practices which indicates **EP-4**.	**Page no:** [19-22] **Section:** [4.1,4.2]

5.	**EP5: Extends of application codes**	No	CO5	N/A	N/A
6.	**EP6: Extends of stakeholders involved and conflicting requirements**	No	CO8	N/A	N/A
7.	**EP7: Interdependence**	Yes	CO5	This project's comprehensive approach addresses high-level problems by integrating various components across data implementation, solving PDE, and proposed methodology, ensuring a holistic solution to complex challenges in Physics-based simulations which ensures **EP-7**.	**Page no:** [25] **Section:** [5.3]

Addressing CO11 with Complex Engineering Activities (EA) [Some or all of the following]:

SN	EA Definition	Attainment	CO	Justification	References
1.	**EA1: Range of resources**	Yes	CO11	Our project utilizes diverse resources such as high-performance computing infrastructure, GPUs, deep learning frameworks, annotated datasets, and ethical considerations to ensure systematic research and contribute to advancements in advancing simulation.	**Page no:** [17] **Section:** [3.3]
2.	**EA2: Level of interaction**	No		N/A	N/A
3.	**EA3: Innovation**	No		N/A	N/A
4.	**EA4: Consequences for society and the environment**	Yes		This project contributes to society by improving simulation condition through advanced PINNs method, while also promoting environmental sustainability by employing efficient computational resources and adhering to ethical guidelines for data privacy.	**Page no:** [25-27] **Section:** [5.1,5.2]

5.	**EA-5: Familiarity**	Yes		This project expands upon existing research by examining a novel approach in Heat transfer simulation through deep learning, demonstrated through preliminary terminologies and a comprehensive comparative analysis, offering new insights into the field.	**Page no:** [10-12] **Section:** [2.2, 2.3]

Addressing CO (4, 9, 10, and 12):

SN	COs	Attainment	Justification	References
1	CO4	Yes	This project addresses **CO4** by integrating effective project management and financial oversight, ensuring meticulous planning, resource allocation, and budget estimation for optimal resource utilization throughout the research lifecycle.	**Page no:** [14] **Section:** [3.0]
2	CO9	Yes	The project demonstrates adherence to ethical principles by prioritizing privacy, obtaining informed consent, and transparently documenting the research process, ensuring responsible knowledge dissemination and societal well-being through the ethical application of advanced healthcare technologies which comply with **CO9**.	**Page no:** [26] **Section:** [5.3]
3	CO10	No	N/A	N/A
4	CO12	Yes	The project's dedication to continuous learning **(CO12)** and adaptation within the dynamic technological landscape is reflected in its comprehensive data collection, rigorous statistical analysis, meticulous methodology development, and thorough experimental results and analysis, showcasing a commitment to staying updated and refining techniques to address modern challenges.	**Page no:** [14-17] **Section:** [3.1, 3.2, 3.3]

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