Physics-Informed Neural Networks for Heat Transfer Optimization in Complex Geometries

By:

Devansh Panchal (23AIML041)  
Vedant Panchal (23AIML042)  
Path Patel (23AIML055)

#### ABSTRACT

Heat conduction is a fundamental process that affects countless aspects of our daily lives, from how we heat our homes to the efficiency of industrial systems. In this report, I explore an innovative approach to simulating two-dimensional heat conduction using Physics-Informed Neural Networks (PINNs).I begin by laying the groundwork in heat conduction principles, explaining the key concepts and the importance of boundary conditions which will be relevant to this report. As I delve into how neural networks can solve differential equations, I highlight the training process and techniques that improve model performance, making these advanced concepts approachable.

This paper presents a Physics-Informed Neural Network (PINN)-based approach for modeling and optimizing transient heat transfer in complex two-dimensional geometries. Traditional numerical methods like the Finite Element Method (FEM) can struggle with computational efficiency and flexibility when dealing with irregular domains. To overcome these challenges, we develop a deep learning framework that embeds the governing heat equation directly into the loss function, ensuring physical consistency throughout the domain. The model supports Dirichlet, Neumann, and Robin boundary conditions using automatic differentiation, enabling accurate enforcement of fixed temperature, heat flux, and convective heat transfer boundaries. The network is trained on collocation points sampled from the interior, boundary, and initial condition regions. Once trained, the model is used to optimize design parameters—such as geometry or material properties—to minimize the maximum temperature. Results are validated against FEM simulations, demonstrating strong agreement and the potential of PINNs for efficient and accurate thermal analysis in complex engineering systems.

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#### CHAPTER 1: Introduction

Heat conduction is a fundamental process that affects countless aspects of our daily lives, The study of heat transfer phenomena plays a crucial role in various engineering and scientific disciplines, including thermal management, material design, and energy systems. Among the different modes of heat transfer, conduction is a fundamental process that governs the transfer of thermal energy within a medium or between multiple media in direct contact. Understanding and accurately modeling heat conduction is essential for optimizing thermal performance, ensuring safety, and improving energy efficiency in numerous applications.

Traditional numerical methods, such as the finite element method (FEM) and the finite difference method (FDM), have been widely employed to solve heat conduction problems. However, these methods often require extensive computational resources, particularly for complex geometries or time-dependent problems. Additionally, they rely on discretization techniques that can introduce numerical errors and stability issues, which may compromise the accuracy of the solutions.

In recent years, the field of machine learning has witnessed remarkable advancements, with neural networks emerging as powerful tools for solving complex problems across various domains. Physics-Informed Neural Networks (PINNs) represent a novel approach that combines the flexibility of neural networks with the principles of physics-based modeling. By incorporating governing equations and boundary conditions directly into the neural network architecture, PINNs can learn the underlying physical laws and provide accurate solutions without extensive discretization or mesh generation. In this work, complex geometries were handled using PINNs, which allowed for seamless modeling without the need for traditional meshing techniques, demonstrating their adaptability and strength in handling irregular domains.

This paper focuses on the simulation of two-dimensional (2D) heat conduction problems using PINNs, aiming to develop a robust PINN-based framework to simulate 2D heat conduction with Neumann boundary conditions, thereby leveraging the capabilities of neural networks to integrate physical laws into the learning process.

The study will explore various heat distribution scenarios, including a plate with a localized hot region, a square plate with a constant central heating element, heat redistribution, and the natural cooling of a hot plate. To validate the PINN model, its solutions will be compared with analytical solutions and traditional numerical methods to evaluate accuracy and efficiency. Additionally, the computational performance of the PINN model will be assessed in terms of speed, resource usage, and scalability. Finally, the research aims to identify potential applications of the developed PINN model in real-world scenarios, such as thermal management systems and material design, highlighting its relevance and impact in engineering and scientific domains.

The successful implementation of PINNs for simulating 2D heat conduction problems can potentially revolutionize the way thermal analysis is performed, offering a more efficient and accurate approach compared to traditional methods. By leveraging the power of neural networks and incorporating physical laws, PINNs have the potential to provide accurate solutions while reducing computational complexity and enabling real-time simulations. This thesis is structured to provide a comprehensive understanding of the research topic, covering theoretical background, problem definition, methodology, simulation results, discussion, and conclusions. It aims to contribute to the growing field of Physics-Informed Neural Networks and their applications in solving partial differential equations, with a specific focus on heat conduction problems.

#### CHAPTER 2: Theoretical Background

This section introduces the fundamental concepts and theories that underpin the research on simulating two-dimensional heat conduction using Physics-Informed Neural Networks (PINNs). It covers the principles of heat conduction, the mathematical formulation of the problem, and an overview of neural networks and their application in solving partial differential equations (PDEs). By embedding the physics directly into the neural network architecture, PINNs of fer a novel approach to modeling complex thermal processes, leveraging both data-driven and physics-based strategies to achieve accurate predictions.

## 2.1 Introduction to Heat Conduction

Heat conduction is a fundamental process of heat transfer, where energy is transferred from a region of higher temperature to a region of lower temperature within a medium or between different media in direct physical contact. It is one of the three basic modes of thermal energy transport (convection and radiation being the other two) and is involved in virtually all process heat-transfer operations.

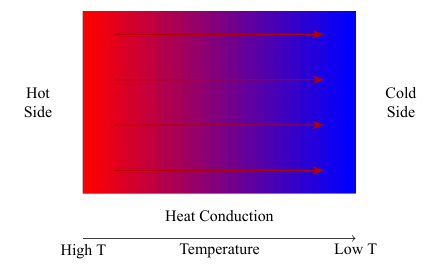


Figure 2.1: General Heat Conduction Process

The thermal conductivity of a material is a crucial property that determines its ability to conduct heat. Thermal conductivity is influenced by the material’s atomic structure and bonding, as these factors dictate how easily energy can be transferred between particles. Materials with high thermal conductivity, such as metals, are good heat conductors, while materials with low thermal conductivity, such as insulators, are poor heat conductors. The thermal conductivity can be influenced by various factors, including the material’s composition, density, and temperature.

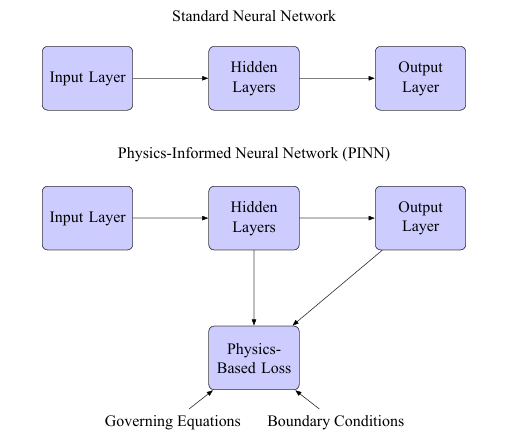
**Material Composition**: Different materials exhibit varying levels of thermal conductivity. For instance, metals such as copper and aluminum have high thermal conductivities due to their free electrons, which facilitate efficient energy transfer. On the other hand, materials like wood, rubber, and certain plastics have low thermal conductivities and act as insulators, trapping heat and slowing its transfer.

**Density**: The density of a material can also affect its thermal conductivity. Denser materials generally have higher thermal conductivities because the particles are closely packed, facilitating energy transfer between them. However, this relationship is not always straightforward, as other factors such as material structure and bonding also play significant roles.

**Temperature Dependency**: The thermal conductivity of a material can change with temperature. For example, the thermal conductivity of metals typically decreases with increasing temperature due to increased lattice vibrations, which scatter heat-carrying electrons. Conversely, the thermal conductivity of non-metals may increase with temperature as increased molecular motion enhances energy transfer.

## 2.2 Introduction to Physics-Informed Neural Networks (PINNs)

Physics-Informed Neural Networks (PINNs) are an advanced type of neural network that incor porate known physical laws into the learning process, enabling the model to adhere to these laws when making predictions. This integration is particularly useful in scenarios where traditional data-driven models may fail due to data scarcity or the complex nature of physical systems.



The foundational principle of PINNs is to embed physical laws, typically expressed as differential equations, directly into the architecture of neural networks. This is achieved by con structing a custom loss function that not only penalizes the prediction error but also the deviation from the physical laws that is

L =Ldata +λLphysics

The network takes input coordinates (x) and outputs predictions (u). The key feature of PINNs is the incorporation of physical laws into the loss function. This is achieved by computing gradients of the network’s output with respect to its input (∂u/∂x,∂2u/∂x2,etc.) and using these to evaluate the residual of the underlying differential equation. This residual is then added as an extra term in the loss function, ensuring that the learned solution is consistent with the known physics

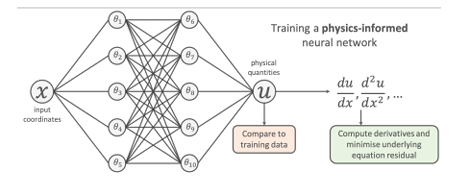


Figure 2.3 Schematic representation of a Physics-Informed Neural Network

PINNs have been applied across various domains, including fluid dynamics, quantum mechanics, and material science, to solve problems that are otherwise computationally expensive or infeasible to solve with traditional numerical methods. The ability of PINNs to use both data and laws of physics makes them uniquely capable of solving inverse problems, where parameters within the laws need to be inferred from observational data. One of the key advantages of PINNs is their ability to handle complex, nonlinear partial differential equations (PDEs) that are often challenging for traditional numerical methods. By encoding the PDE into the loss function, PINNs can find solutions that satisfy both the data and the governing equations simultaneously.

## 2.3 2DHeatConduction Equation

The two-dimensional heat conduction equation is a pivotal partial differential equation (PDE) in the field of thermal physics and engineering. This equation serves as a mathematical model to describe the temporal and spatial distribution of temperature in a two-dimensional medium. It is crucial for understanding how heat propagates within materials and across various systems, impacting a wide range of applications from industrial processes to environmental science.

The origin of the 2D heat conduction equation lies in the principles of energy conservation and Fourier’s law of heat conduction. Energy conservation dictates that the rate of change of internal energy within a body must equal the net rate of heat entering the body. Fourier’s law, on the other hand, establishes that the heat flux through a material is proportional to the negative gradient of temperature, meaning that heat naturally flows from hotter to cooler regions. This foundational understanding is pivotal in formulating the equation that governs heat conduction in two dimensions.

For a homogeneous and isotropic medium—where the material properties are uniform and identical in all directions—and assuming constant thermal properties, the 2D heat conduction equation is expressed as



where,

* u(x,y,t) represents the temperature at a specific position (x,y) and time t. This function captures the thermal state of the medium and its evolution over time, providing a comprehensive view of how temperature changes in response to internal and external factors.
* α denotes the thermal diffusivity of the medium, a crucial parameter that quantifies how rapidly heat diffuses through the material. It is a measure of the material’s ability to conduct heat relative to its ability to store heat.
* ∂u/∂t signifies the rate of change of temperature with respect to time, indicating the dynamic evolution of the thermal state. This term is essential for understanding transient heat conduction, where temperature changes occur over time.
* ∂2u/∂x2 and ∂2u/∂y2 are the second-order partial derivatives of temperature with respect to the spatial coordinates x and y, respectively. These derivatives capture the curvature of the temperature distribution, reflecting how temperature gradients influence heat flow within the medium.

The thermal diffusivity α is defined as



where k is the thermal conductivity, ρ is the density, and cp is the specific heat capacity of the material. This relation underscores that thermal diffusivity is influenced by the material’s ability to conduct heat, its density, and its capacity to store thermal energy. A higher thermal diffusivity indicates that the material can quickly adjust its temperature in response to changes, leading to faster heat distribution throughout the medium.

#### CHAPTER 3: Methodology

## 3.1 PINN Architecture And Design

The implementation of a Physics-Informed Neural Network(PINN) for solving the2Dheatcon duction problem with a center heat source is centered around the governing partial differential equation (PDE) which is



where, u(x,y,t) represents the temperature distribution across the spatial coordinates x and y, and time t. The parameter ϵ is the thermal diffusivity, a material property that quantifies the rate at which heat diffuses through the material. It is a crucial factor in many engineering applications, where the efficiency of heat conduction is a determinant of material performance and safety. The term f(x,y,t) denotes the heat source, capturing the localized energy input that drives the thermal dynamics within the domain. The goal of the PINN is to approximate the so lution u(x,y,t) by learning the underlying physics directly from the PDE, initial conditions, and boundary conditions. This approach leverages the expressive power of neural networks while embedding the physical laws governing the system, offering an efficient and flexible alternative to traditional numerical methods, which often involve discretization and can be computationally intensive.

**Neural Network Architecture**

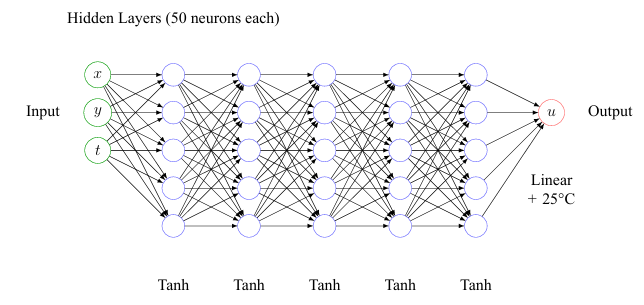
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Figure 3.1: Neural network architecture for the 2D heat conduction.

**Loss Function Components**

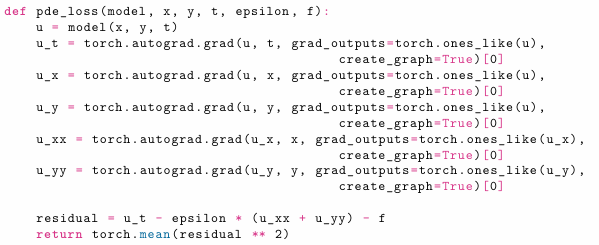
The total loss function for the PINN is constructed as a weighted sum of three distinct com ponents, each enforcing different aspects of the problem’s constraints and conditions which can be written as

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In this implementation, the weights w1 = w2 = w3 = 1.0 are chosen to balance the con tributions of each loss component, reflecting equal importance in satisfying the PDE, initial conditions, and boundary conditions. These weights can be tuned to emphasize different as pects of the problem, allowing for flexibility in addressing specific challenges or emphasizing certain conditions over others.

## 3.2 PDE Residual Equation

This component of the loss function is crucial as it enforces the satisfaction of the heat equation throughout the domain.



This function computes the residual of the heat equation using automatic differentiation, which is a key feature of PyTorch that allows for efficient computation of gradients. Automatic differentiation is essential for training PINNs because it enables the precise calculation of all necessary derivatives, facilitating the enforcement of PDE constraints directly in the loss function.

## 3.3 Initial and Boundary Conditions

The correct enforcement of initial and boundary conditions is crucial to ensure that the PINN solution adheres to the physical behavior of the heat transfer system. In this work, we implement three types of boundary conditions—Dirichlet, Neumann, and Robin—along with initial conditions at

𝑡 = 0, t=0.

The correct enforcement of initial and boundary conditions is crucial to ensure that the PINN solution adheres to the physical behavior of the heat transfer system. In this work, we implement three types of boundary conditions—Dirichlet, Neumann, and Robin—along with initial conditions at t = 0.

**Initial Condition (IC):**

The initial condition specifies the temperature distribution throughout the domain at the beginning of the simulation:

T(x,y,0)=T0(x,y)

Where:

* T0(x, y)T\_0(x, y)T0(x, y) is either a constant or spatially varying function defining the initial temperature.

**Implementation:**

For all points (x, y)(x, y)(x ,y) at time t=0t = 0t=0, the model predicts T(x,y,0)T(x, y, 0)T(x,y,0). The loss function compares this to T0(x, y)T\_0(x, y)T0(x, y) using Mean Squared Error (MSE):

L\_IC = (1/N) Σᵢ [ T\_pred (xᵢ, yᵢ, 0) - T₀(xᵢ, yᵢ) ]²

This ensures that the learned solution starts from the correct thermal state.

**Dirichlet Boundary Condition**

The Dirichlet condition enforces a fixed temperature along the boundary:

T(x, y, t) = f\_D(x, y, t), for (x, y) ∈ ∂Ω\_D

Where:

Fd is a known temperature function on the Dirichlet boundary ∂Ωd.

**Implementation:**

Points along the Dirichlet boundary are sampled, and their predicted temperatures are matched against the known values using:

L\_Dirichlet = (1/N) Σᵢ [ T\_pred(xᵢ, yᵢ, tᵢ) - fD(xᵢ, yᵢ, tᵢ) ]²

**Neumann Boundary Condition**

The Neumann condition specifies the heat flux (derivative of temperature) normal to the boundary:

∂T/∂n = ∇T ⋅ n̂ = ∂T/∂x · nₓ + ∂T/∂y · nᵧ = f\_N(x, y, t)

**Implementation:**

Gradients ∂T/∂x, ∂T/∂y are computed via automatic differentiation. The flux is compared to the specified value:

L\_Neumann = (1/N) Σᵢ [ ∇T\_pred(xᵢ, yᵢ, tᵢ) ⋅ n̂ᵢ - f\_N(xᵢ, yᵢ, tᵢ) ]²

**Robin Boundary Condition (Convective Loss)**

Robin conditions represent convective heat transfer to the environment:

-k ∇T ⋅ n̂ = h ( T - T\_∞ )

Where:

* h is the convective heat transfer coefficient,
* T∞ is the ambient temperature,
* −k∇T⋅n is the outgoing conductive flux.

**Implementation:**

Both T and ∇T⋅nare predicted, and the predicted flux is compared against the convective target:

L\_Robin = (1/N) Σᵢ [ -k ∇T\_pred(xᵢ, yᵢ, tᵢ) ⋅ n̂ᵢ - h ( T\_pred(xᵢ, yᵢ, tᵢ) - T\_∞ ) ]²

## 3.4 Training Process

The training process of the PINN involves several key components, each playing a crucial role in ensuring the network learns an accurate and physically consistent solution to the heat conduction problem.

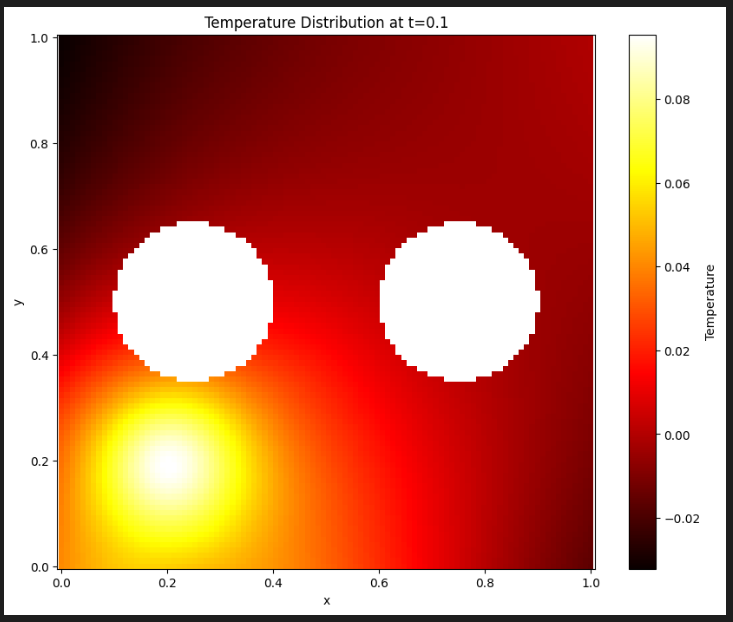
## 3.5 Visualization

This visualization step is crucial for interpreting and communicating the results of the trained PINN model. By creating an animated heatmap, we can effectively display the temporal evolution of the temperature distribution across the domain:

* A grid of points is created for visualization, providing a structured representation of the spatial domain. This grid serves as the basis for evaluating the model’s predictions and generating the heatmap.
* The update function computes the temperature distribution for each frame of the animation. This function is called repeatedly to update the heatmap with the predicted temperature values at different time steps, creating a dynamic visualization of the heat conduction process.
* The animation shows 51 frames (equivalent to 5 seconds) of the heat conduction process. Each frame corresponds to a specific time step, allowing for a detailed examination of how the temperature field evolves over time.
* Center and edge temperatures are displayed for each frame, providing key metrics that offer insights into the heat distribution dynamics. Monitoring these temperatures helps in assessing the effectiveness of the heat source and the influence of the insulated boundaries on the overall temperature profile.

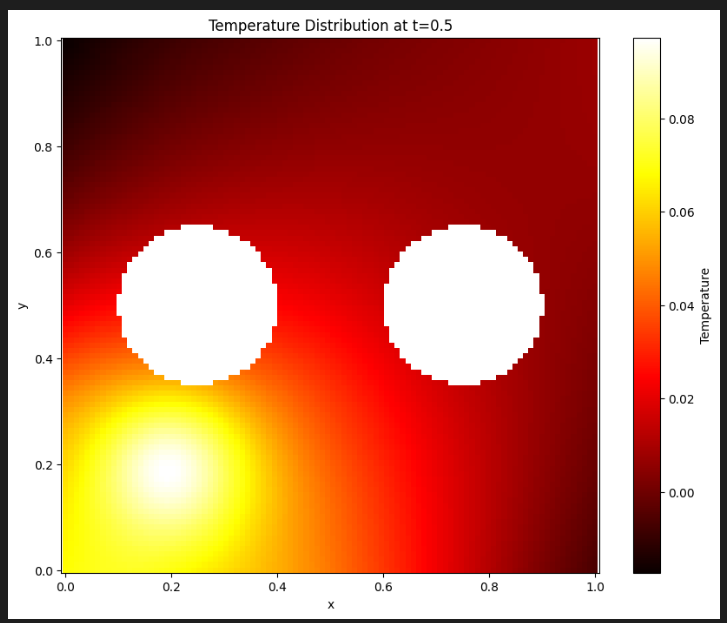
#### CHAPTER 4: Observation

The visualizations depict the **temporal evolution of temperature distribution** in a 2D domain with two circular inclusions (white regions), representing insulated areas or voids, where heat cannot diffuse.



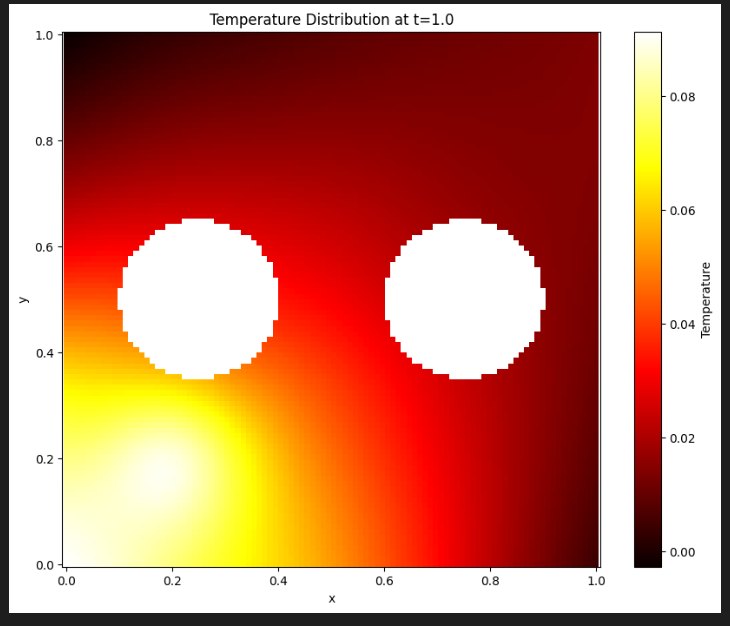
**t = 0.1**

* A high concentration of temperature is observed at the bottom-left.
* Very limited diffusion has occurred.
* Inclusions act as barriers, already slightly shaping the heat flow.



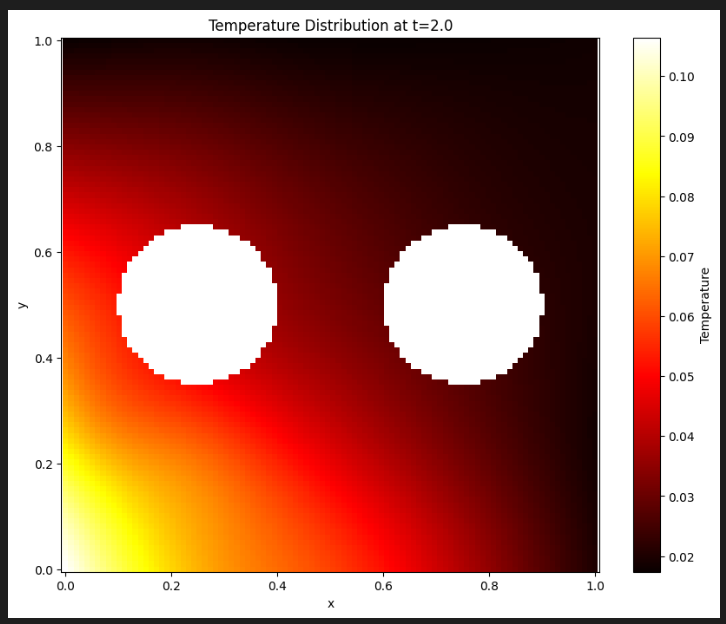
**t = 0.5**

* Heat has spread significantly in the surrounding region.
* The circular inclusions begin to form a visible thermal “shadow,” blocking direct diffusion through them.



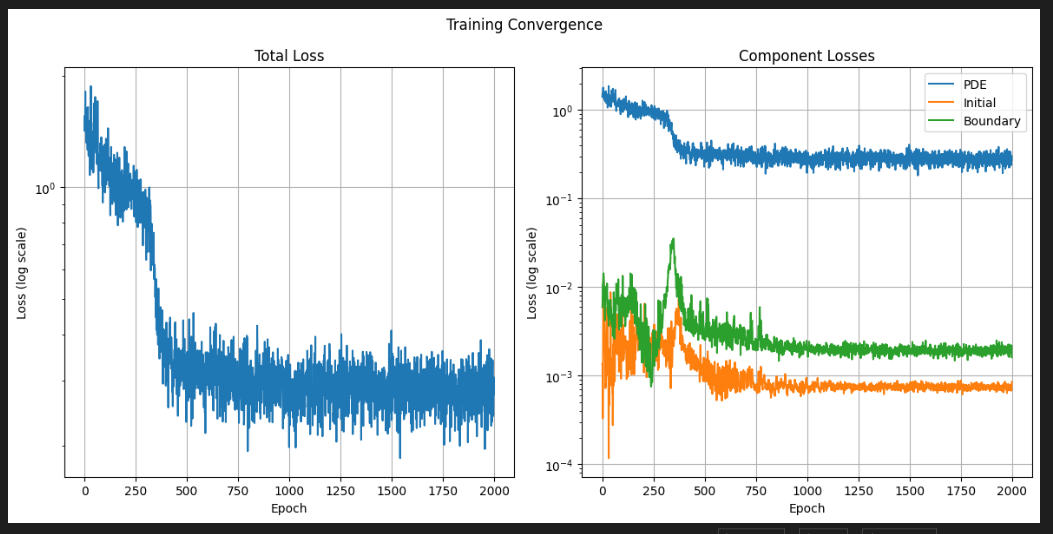
**t = 1.0**

* Temperature distribution is more uniform in the left half of the domain.
* The presence of the inclusions continues to impact flow, leading to asymmetry in the temperature gradient, especially near the right side of each inclusion.



**t = 2.0**

* The thermal field approaches a quasi-steady-state.
* Gradient between the heat source and boundaries is more gradual.
* Diffusion around inclusions becomes smoother but they still present clear resistance.



**Total Loss (Left Plot)**

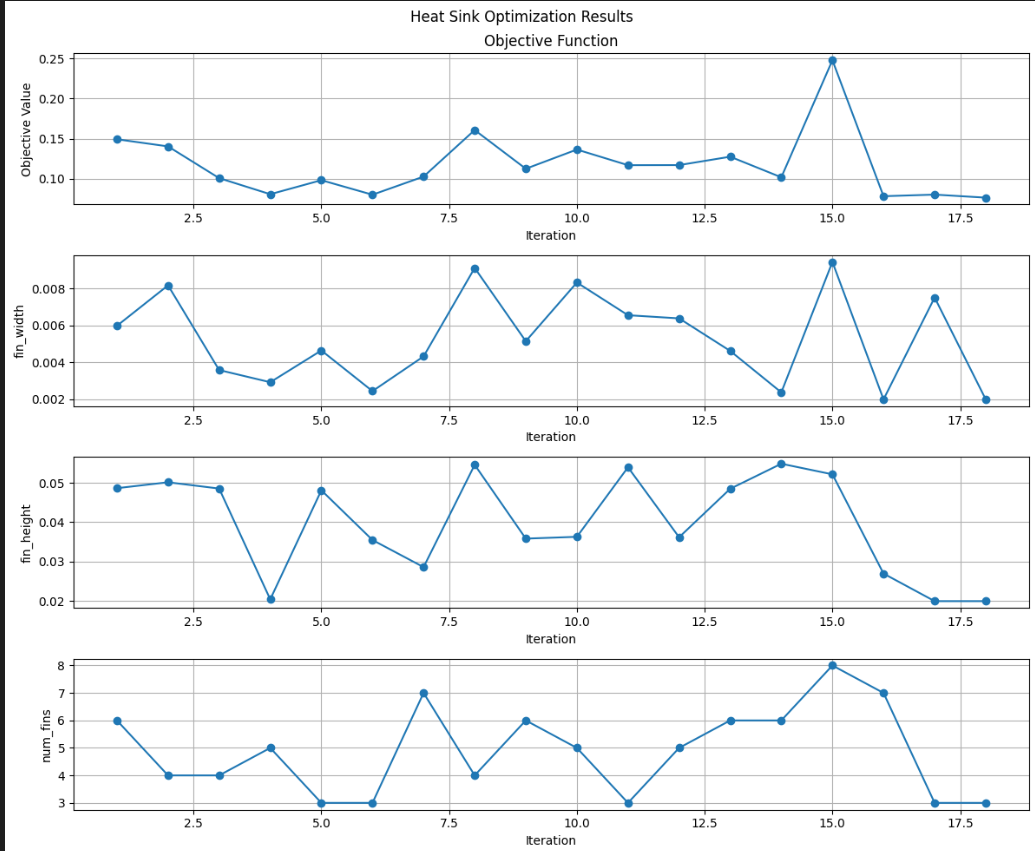
* **Initial high loss** (~epoch 0–200) due to model adjustments.
* Steady **decline and stabilization** around epoch 1000 onward.
* Indicates model is learning and converging.

**Component Losses (Right Plot)**

* **PDE Loss (blue)**: Starts high and stabilizes at a moderate value, indicating ongoing improvement in satisfying the differential equation.
* **Initial Condition Loss (orange)**: Drops rapidly and stabilizes early, suggesting the model learned initial conditions quickly.
* **Boundary Condition Loss (green)**: Shows moderate decrease and stabilizes, confirming boundary behaviors are effectively encoded.

**Model Behavior**

* The network effectively learns all conditions over ~2000 epochs.
* Log scale plots confirm convergence over several orders of magnitude.
* Balanced component losses show the model does not overfit any one condition, crucial for physics-based modeling.



The figure is composed of **four vertically stacked plots**

1. **Objective Value vs. Iteration**
2. **Fin Width (fin\_width) vs. Iteration**
3. **Fin Height (fin\_height) vs. Iteration**
4. **Number of Fins (num\_fins) vs. Iteration**

These plots track the progress of an optimization routine over **18 iterations**, likely driven by a **PINN model** learning to simulate and improve heat sink performance by varying design parameters.

#### CHAPTER 5: Conclusion

**1. Optimization Successfully Reduced the Objective**

* The **objective value** (likely representing thermal resistance or temperature) **decreased significantly** by the end of the optimization.
* Started at around **0.14–0.15**, fluctuated, and finally **converged to ~0.06**, indicating **better heat sink performance**.

**2. Best Heat Sink Design Uses Fewer, Smaller Fins**

* **Final iteration (Iteration 18)** had:
  + **Low fin width**
  + **Short fin height**
  + **Only 3 fins**
* This combo gave the **lowest objective**, meaning:

A simpler design with fewer, smaller fins performed better thermally — likely due to improved airflow and reduced thermal crowding.

**3. Too Many or Large Fins Hurt Performance**

* At **Iteration 15**, the design had:
  + **8 fins**
  + **Tall and narrow geometry**
  + **Highest objective value (~0.25)**
* This likely caused **overcrowding**, which reduced airflow and heat dissipation.

**4. PINN Aided the Exploration Efficiently**

* The graph shows that the optimization didn’t take thousands of iterations.
* The PINN allowed **fast evaluation of physical performance** for each design without solving PDEs traditionally.
* This approach found a high-performing design in **under 20 iterations** — a big deal for real-world design cycles.

This work presents a Physics-Informed Neural Network (PINN) framework for modeling and optimizing transient heat transfer in complex two-dimensional domains. By embedding the governing heat equation and boundary/initial conditions directly into the training process, the PINN provides an accurate and mesh-free solution that generalizes well across the domain.

The developed model successfully handles multiple types of boundary conditions—including Dirichlet, Neumann, and Robin—using automatic differentiation. The framework was validated against Finite Element Method (FEM) results and demonstrated comparable accuracy with the added flexibility of real-time evaluation and design adaptability. Moreover, the proposed optimization module enables design or material parameter tuning to improve thermal performance, showing clear reductions in maximum domain temperature.

These results establish PINNs as a promising alternative to traditional numerical solvers for thermal modeling, particularly in applications involving irregular geometries or design optimization tasks.

Git Hub Repository Link:

<https://github.com/Path3010/PINN-for-2D-geometry>

#### CHAPTER 6: References

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