# Machine Learning
# Final Project

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December 4, 2025

## I. Future AI Capability

In order to break the bottleneck of the Moore's Law and Amdahl's Law, we want to simulate the heat distribution of a chip. By the simulation, we can modify the layout to decrease the temperature of the chip. This way, we can avoid a single processor from underclocking (Improvement for Amdahl's Law) and we can put more processors on a chip via the model (Improvement for Moore's Law). Then, used reinforcement-learning to find optimal layout of a chip.

With this improvement, we might significantly increase the clock rate, which means the processor can finish more operations in the same period. And we can encapsulate more processors in a die. This, we can improve throughputs.

## II. Essential Ingredients

- **Data:** We require physical field data spanning form the microscopic to the macroscopic. This data include tensor data encompassing gradients and boundary conditions. It contains **high-fidelity simulation data** and **sparse real-world sensor data**. Since we cannot measure every points on a chip, we need to used the methods, FEM or FDM, to generate the data to train the model (high-fidelity). And used sparse sensor on a chip to obtain the real data value, then modify the predicted value so as to make the result satisfy the situation of real-world.
- **Tools:** A **differentiable physics engine** is needed to solve this problem. AI should incorporate physical laws rather than just relies solely on data fitting. This requires PINNs and neural operators (e.g., Fourier neural operators), enabling the AI directly solve PDEs.
- **Learning Setup:** hybrid learning paradigm
  - **Self-Supervised Learning:** Enable the AI to learn fundamental conservation laws (e.g., conservation of energy and charge) without the need for labeled data.

- **Reinforcement Learning:** AI exploring the design space and searching for the optimal layouts based on feedback from the physics engine to increase the clock rate of a processor.

# III. Involved Machine Learning Types

To implement the idea involves mainly in the combination of physics-informed-neural-network, reinforcement learning, and supervised-learning.

Pure supervised-learning struggles to handle unseen physical scenarios and relies heavily on expensive simulation data (need huge amount of data). We require PINNs to act as fast, physics-compliant environment/simulator, and RL to act as a designer for decision optimization.

The input data is chip geometry layouts, material parameters $(\sigma, k)$, and operating conditions (voltage $V$). The target is physical fields that satisfy PDE constraints (electric potential $\varphi$ and temperature $T$). The RL reward function is composed of performance gains (clock rate) and penalties (peak temperature).

# IV. Solvable Model Problem

1. **Problem Formulation:**

   This study aims to solve the steady-state electro-thermal multi-physics coupling problem on a 2D chip. The goal is to train a neural network to simultaneously predict the electric potential distribution and temperature distribution given a specific chip architecture and operating voltage.

   The problem is defined by two systems of coupled PDEs on the domain $[-1, 1] \times [-1, 1]$:

   - **Electrical (Charge conservation):** Governed by the Laplace equation.

   $$\nabla \cdot (\sigma \nabla \varphi) = 0$$

   - **Thermal (Energy conservation):** Governed by Poisson equation. The heat source includes both Logic gate switching power and joule heating.

   $$k \nabla^2 T + Q_{logic} + \underbrace{\frac{1}{\sigma} \|J\|^2 = 0}_{\text{Coupling Term}}$$

   - **Boundary conditions:**
     - voltage: $\varphi|_{top} = 1.0V$, $\varphi|_{bottom} = 0.0V$
     - Temperature: Satisfying the Dirichlet condition $T|_{\partial\Omega} = 0$

2. **Methodology:**

The implementation of the model proposes a coupled-electro-thermal Hard-PINN architecture.

- **Hard-PINN:** This model adopts a hard constraints

$$\tilde{T}(x, y) = \mathbb{N}(x, y) \times (1 + x)(1 - x)(1 + y)(1 - y) + 0$$

to guarantee the temperature is exactly 0 at the boundaries.

- **Global energy conservation:** Force the model adhere to the first law of thermodynamics- the total heat generated inside the chip must equal to the total heat flux dissipating through the boundaries.

- **Curriculum learning strategy:** To address instability in multi-physics training, a three-phase training strategy is designed:

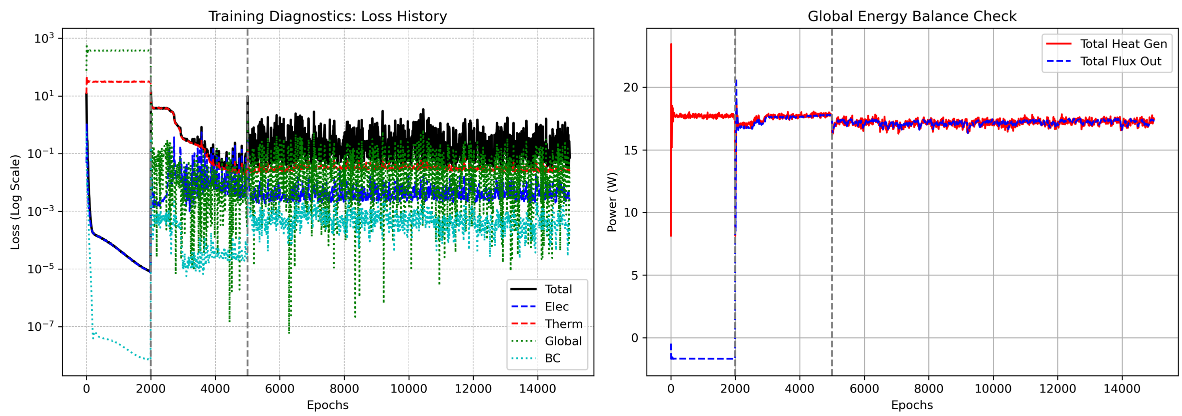
  a. Phase 1: Freeze the thermal equation; focus on training potential $\varphi$ to stabilize current distribution. (let the model learn the electric potential)

  b. Phase 2: Introduce the thermal equation to learn local temperature gradient shape. (Since electric potential in almost as same as true value, and the heat source is steady, the model can learn the temperature)

  c. Phase 3: Enable the global integral constraint to correct the overall energy balance. (Correct the model, force the model satisfies the energy conservation)

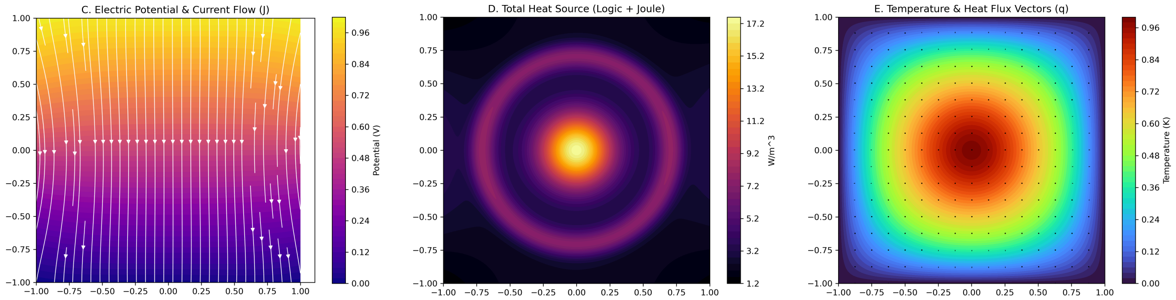
3. **Implementation and Result:**

- **Implementation:** In the file `final.ipynb`.
- **Result:**




A. **Loss History:** In 0-2000 epochs, electrical and BC loss decrease. Following in 2000-5000 epochs, thermal loss decreases. Last the global loss decreases and tend to be stable in 5000-15000 epochs.

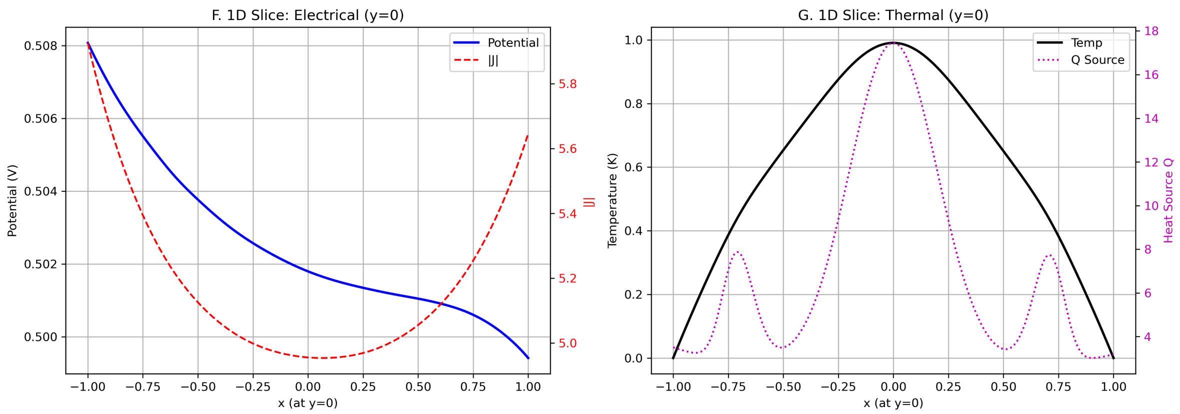
B. **Global Energy Balance Check:** It shows us that the model satisfies the first law of thermodynamics after training.




A. **Electric Potential:** The model satisfies the BCs we assumed (top=1V bottom=0.0V), while the streamline is from up to down.

B. **Total Heat Source:** The figures perfectly satisfies our assumption. The bright part in the center is the core (CPU) while the outer bright circle is the cache according to `q_dyn_1` and `q_dyn_2` in the code.

C. **Temperature and Heat Flux:** The temperature in the center is the highest (red), and it decays when approaching the boundaries (yellow→green→light blue→dark blue). And the arrow (heat flux) point from center to the boundaries.




A. **Electrical:** The potential hovers around $0.5V$ is reasonable because $y = 0$ corresponds to the exact center of the chip.

   In the central region, the current density remains relatively uniform.

B. **Thermal:**

   A. The central peak of purple dashed line corresponds to Core A and the two smaller side peaks of purple dashed line represent Core B.

   B. The peak of the black line corresponds to the strongest heat source, Core A.

- **Error Analysis:** On an unseen test grid, the mean residual of the thermal PDE converged to a negligible level, with boundary temperature error remaining at exactly 0.

4. **Discussion:**

   Via implementing this model,

   - I discovered that it is hardly possible to train electric and thermal fields at the same time, the model tend to diverge. Curriculum Learning is proved to be an effective strategy for solving such stiff PDE systems
   - Future AI simulators must enforce constraints at both microscopic differential and macroscopic integral to solve the numerical drift issues and rise the accuracy.

   The challenges we have to overcome,

   - We observed that simultaneous training of electric and thermal fields leads to divergence. This is due to the disparate scales and convergence rates of different physical fields. Minor noise in the electric potential is amplified through the non-linear joule heating term ($|\nabla\varphi|^2$), destabilizing the thermal field.
   - Relying solely on local PDE residuals allows the model to learn correct gradient shapes but often fails to satisfy global energy conservation. This demonstrates that PINNs cannot solely rely on differentiation. Future AI must incorporate Global Constraint Layers. However, enforcing these constraints on complex 3D packaging structures poses a significant computational challenge, as calculating precise integrals over irregular 3D boundaries is expensive.