Optimizing LIG Formation on Polyimide Surfaces Using DL

Leveraging Physics-Informed Neural Networks (PINNs) for Predictive Modeling and Process Optimization

Arka Mukherjee

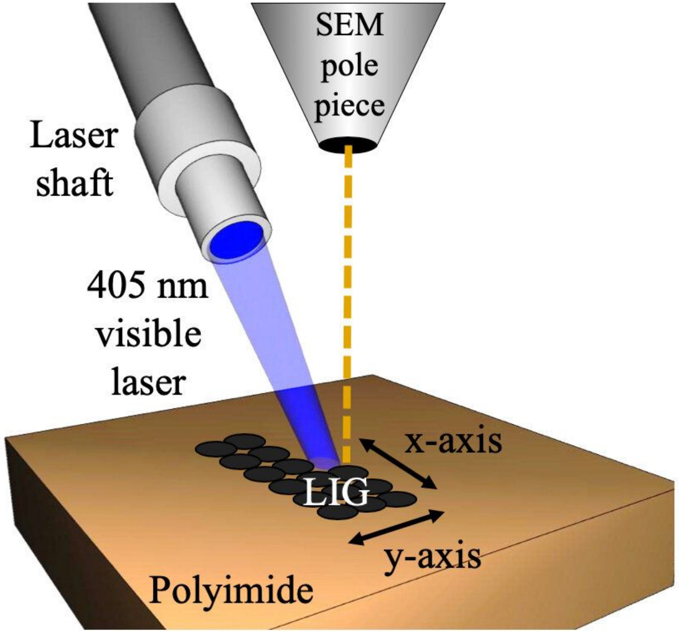
Introduction to Graphene and LIG Process

Overview of Graphene:

- Structure: 2D sheet of carbon atoms in a honeycomb lattice.
- Unique properties: Electrical conductivity, mechanical strength, flexibility.

Laser-Induced Graphene (LIG) Formation:

- Laser interaction with polyimide to create graphene.
- Importance for flexible electronics, sensors, energy storage.

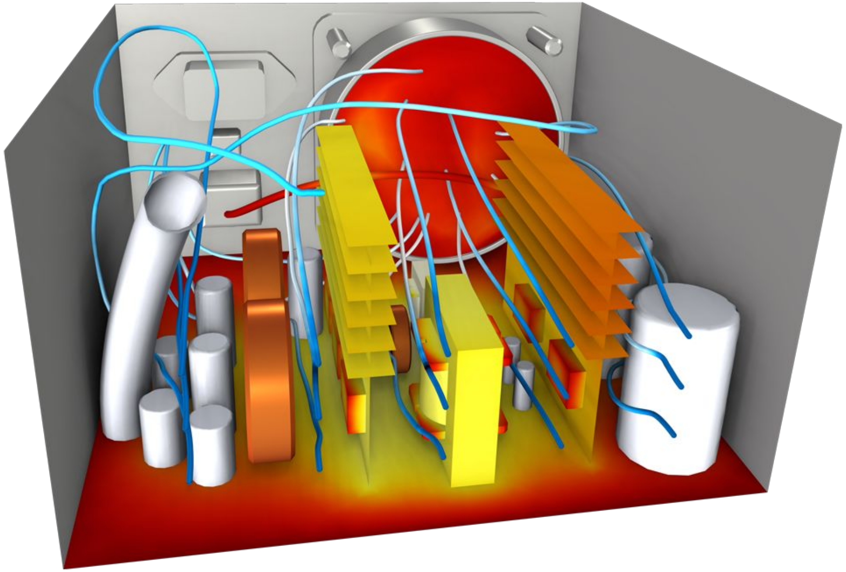


Limitations of Traditional Simulation Tools (COMSOL)

Challenges in COMSOL:

- Simplified assumptions in modeling heat transfer and chemical reactions.
- Inaccurate representation of thermal and optical interactions.
- Difficulty modeling nonlinear behaviors during laser-polyimide interaction.
- Incomplete multiphysics coupling (heat, phase changes, chemical reactions).

Impact: Discrepancies between simulated and experimental results, making it hard to predict optimal laser parameters and surface conditions.



Objectives and Problem Statement

Objective:

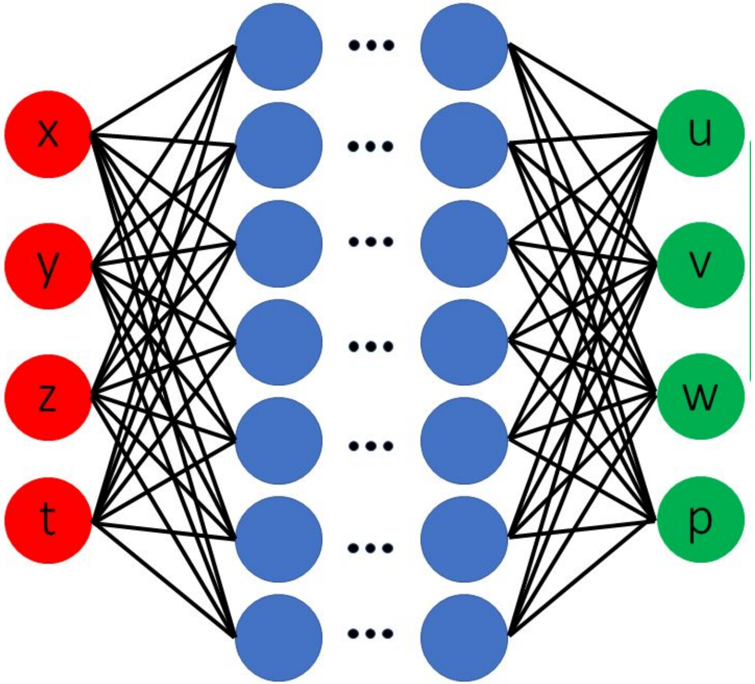
- Develop a **deep learning-based model (PINN)** that accurately predicts critical laser parameters and surface properties for high-quality graphene formation.

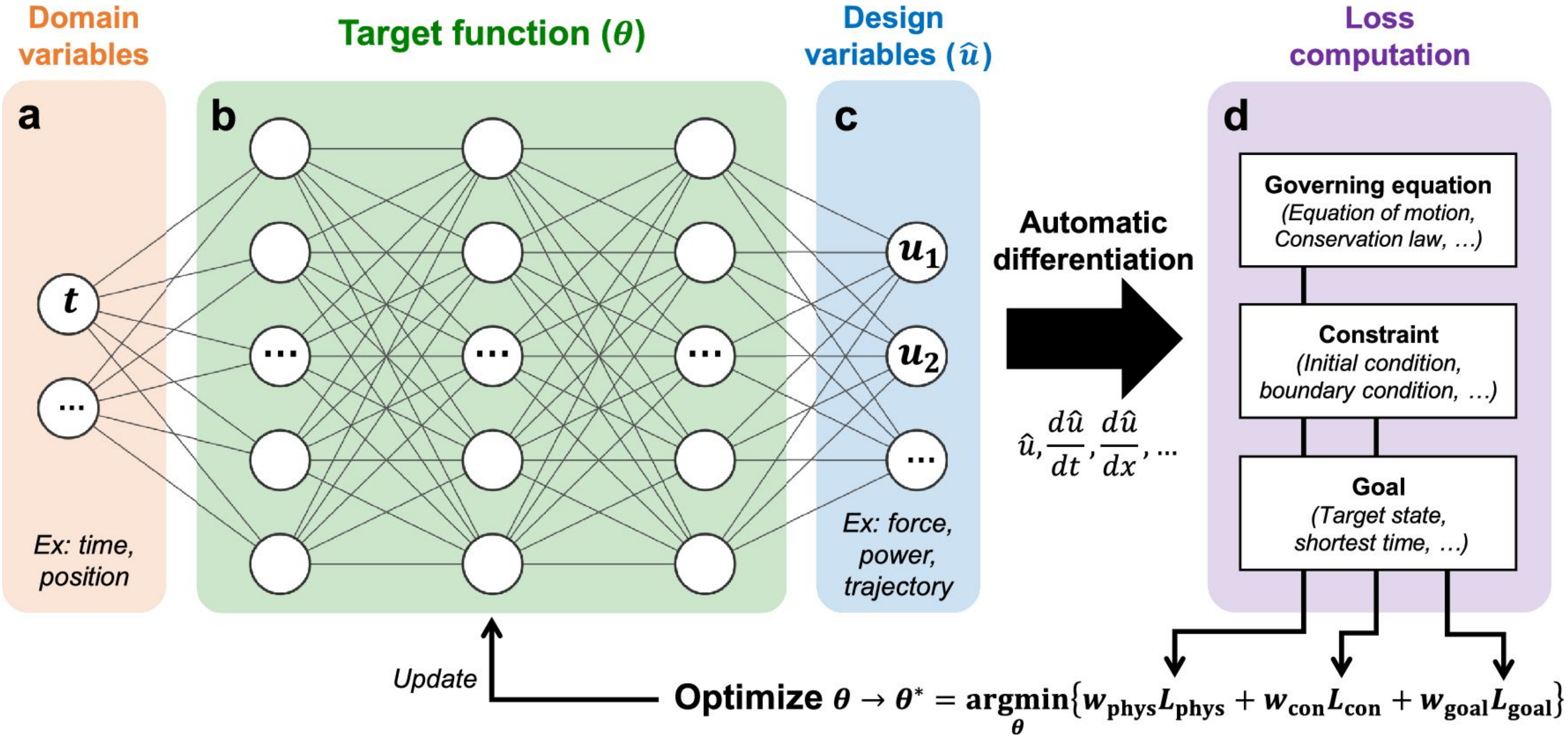
Problem:

- Traditional tools cannot handle complex, nonlinear **interactions and material responses** during the LIG process.

Goal:

- Overcome COMSOL's limitations with PINNs, leading to better accuracy in predicting optimal graphene formation conditions.





Domain variables
Target function (θ)
Design variables ($\hat{u}$)
Loss computation
a
b
c
d
t
...
Ex: time, position
u_1
u_2
...
Ex: force, power, trajectory
Automatic differentiation
$\hat{u}, \frac{d\hat{u}}{dt}, \frac{d\hat{u}}{dx}, \ldots$
Governing equation
(Equation of motion, Conservation law, …)
Constraint
(Initial condition, boundary condition, …)
Goal
(Target state, shortest time, …)
Update
Optimize $\theta \rightarrow \theta^* = \underset{\theta}{\operatorname{argmin}}\{w_{\text{phys}}L_{\text{phys}} + w_{\text{con}}L_{\text{con}} + w_{\text{goal}}L_{\text{goal}}\}$

PINNs Approach for LIG Optimization

What Are PINNs:

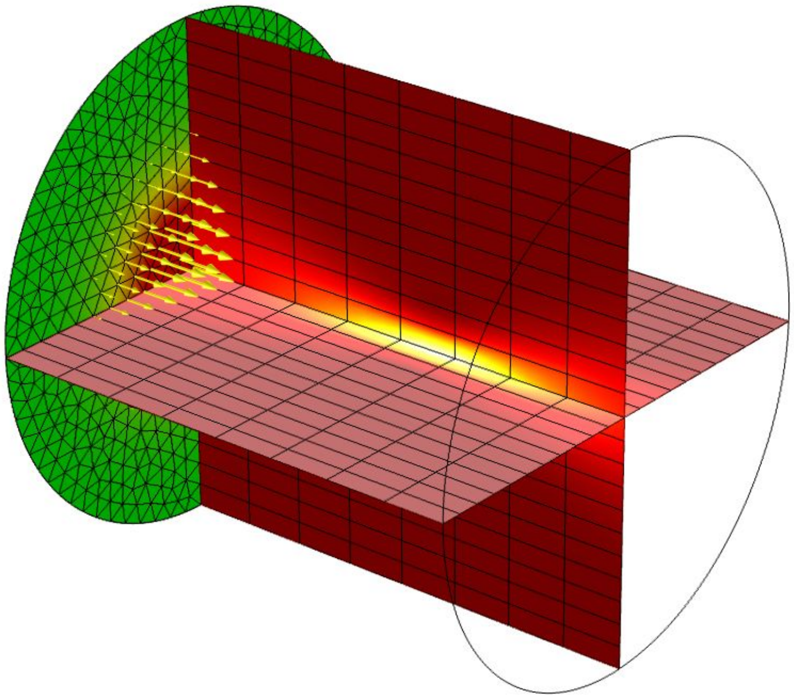
- Neural networks informed by physical laws (e.g., thermodynamics, heat transfer) integrated with data-driven methods.

How PINNs Solve the Problem:

- Incorporate governing equations of **laser-material interaction**.
- Handle nonlinearities and complex multiphysics coupling (**heat diffusion, chemical reactions**).
- Use both experimental and simulation data for training.

Advantages Over Traditional Methods:

- Better prediction accuracy for laser parameters and graphene quality.
- Real-time learning and adaptation to material and process variations.



Expected Outcomes and Applications

Expected Outcomes:

- A robust model capable of **predicting optimal laser conditions and polyimide surface properties** for high-quality graphene formation.
- Improved **efficiency, reduced costs, and scalability of LIG processes** for industrial applications.

Applications:

- Flexible electronics, wearable sensors, energy storage devices, advanced nanocomposites.

Next Steps:

- Implement PINN model, validate with experimental data, and optimize for industrial scalability.