Physics-Informed Neural Networks for Heat Transfer Predictions in Additive Manufacturing

Junhyeok Kil

Akshay Jacob Thomas, Ph.D.

Eduardo Barocio, Ph.D.

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May 20, 2025

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Conference & Exhibition
May 19-22, 2025 | Indianapolis, Indiana

About

- Junhyeok Kil (kilj@purdue.edu)
- Purdue Department of Computer Science
- Undergraduate Research Assistant
- Composites Manufacturing & Simulation Center
- Supervisor: Eduardo Barocio, Ph.D.

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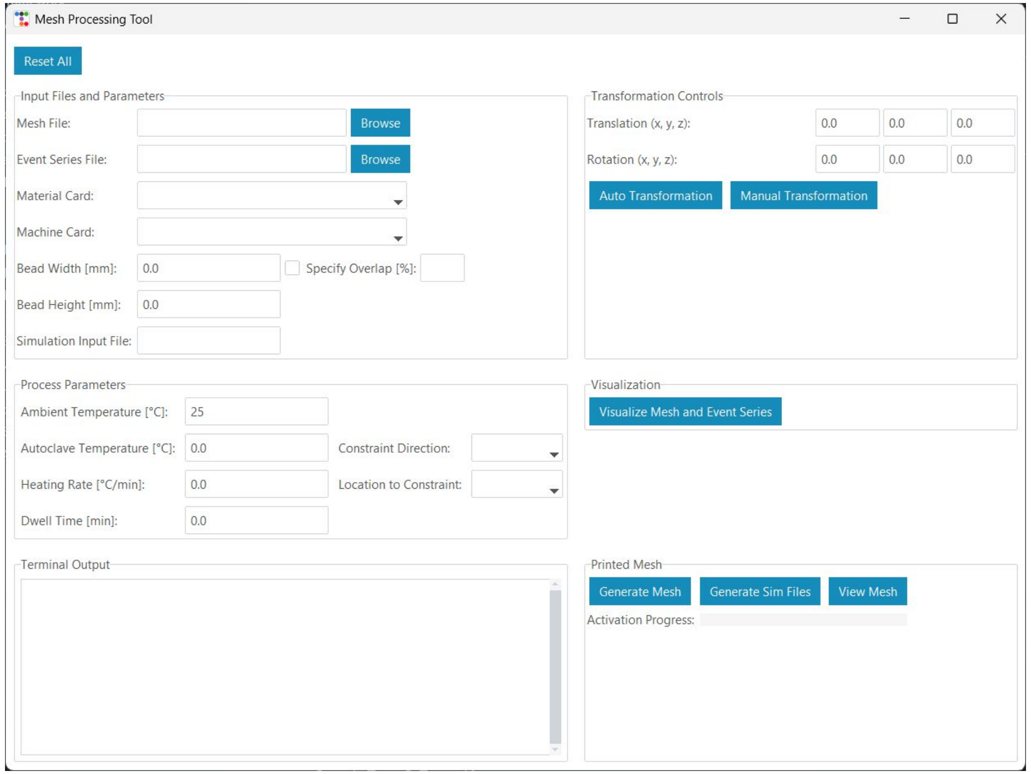
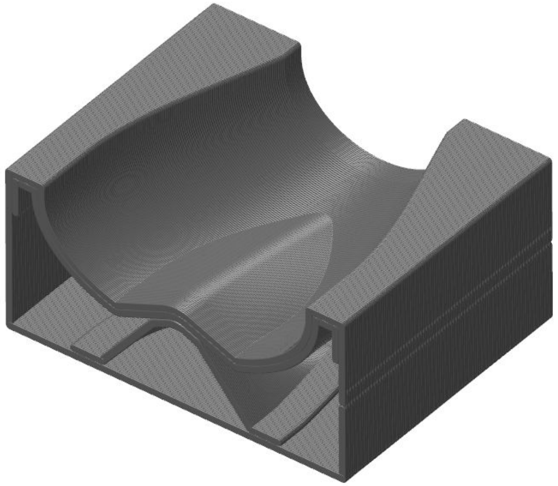
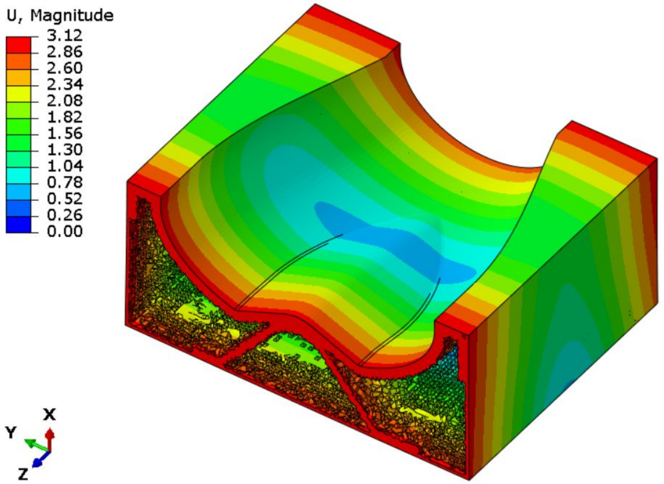
Other Research Projects



Graphical User Interface



LSAM Tool Design



Shape Compensation of LSAM Tool Design

Thermwood LSAM Research Laboratory at Purdue

Goal: Support Thermwood and the Large-Scale Additive Manufacturing industry by delivering applied research and physics-based process simulations.

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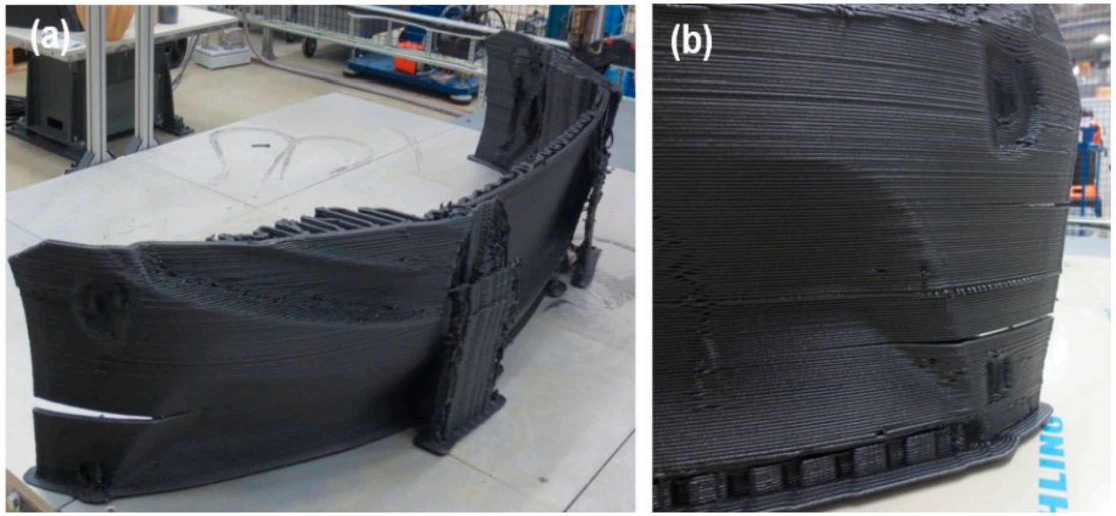
Large-Scale Additive Manufacturing

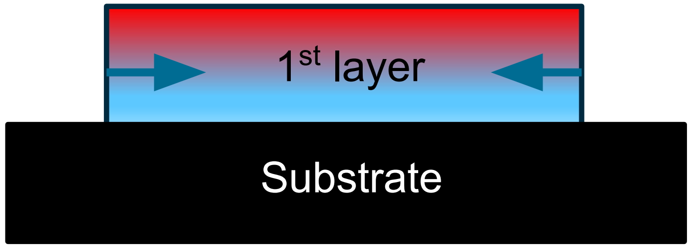
Potential Challenges



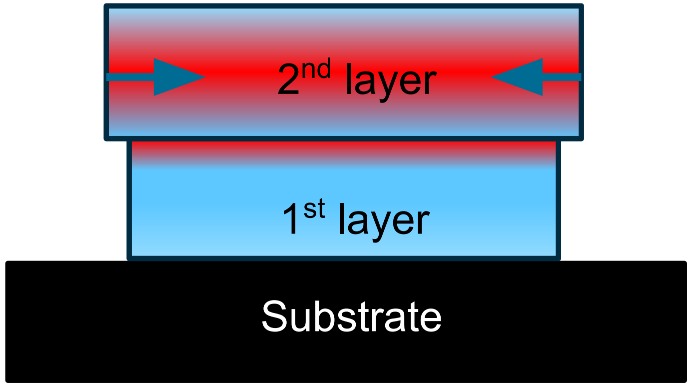
Akbari, S., Johansson, J., Johansson, E., Tönnäng, L., & Hosseini, S. (2022). Large-Scale Robot-Based Polymer and Composite Additive Manufacturing: Failure Modes and Thermal Simulation. *Polymers*, *14*(9), 1731. https://doi.org/10.3390/polym14091731
L. J. Love, “Utility of big area additive manufacturing (BAAM) for the rapid manufacture of customized electric vehicles,” Oak Ridge National Laboratory (ORNL); Manufacturing Demonstration Facility (MDF), 2015.

Predicting Thermal History

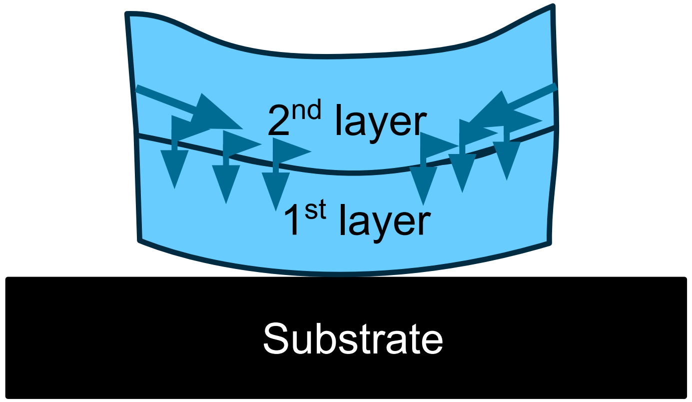
Thermal contraction



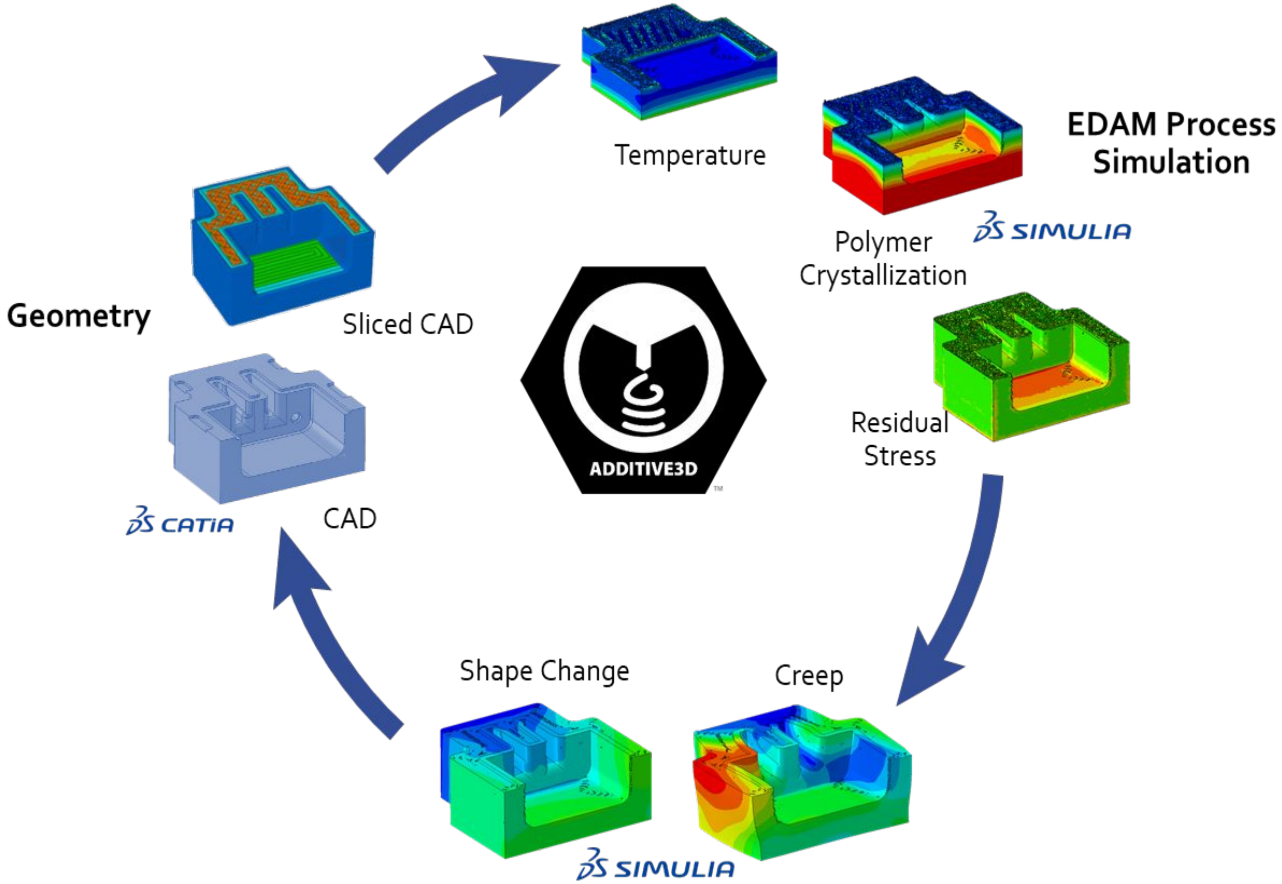
New hot layer placed on contracted cooled layer



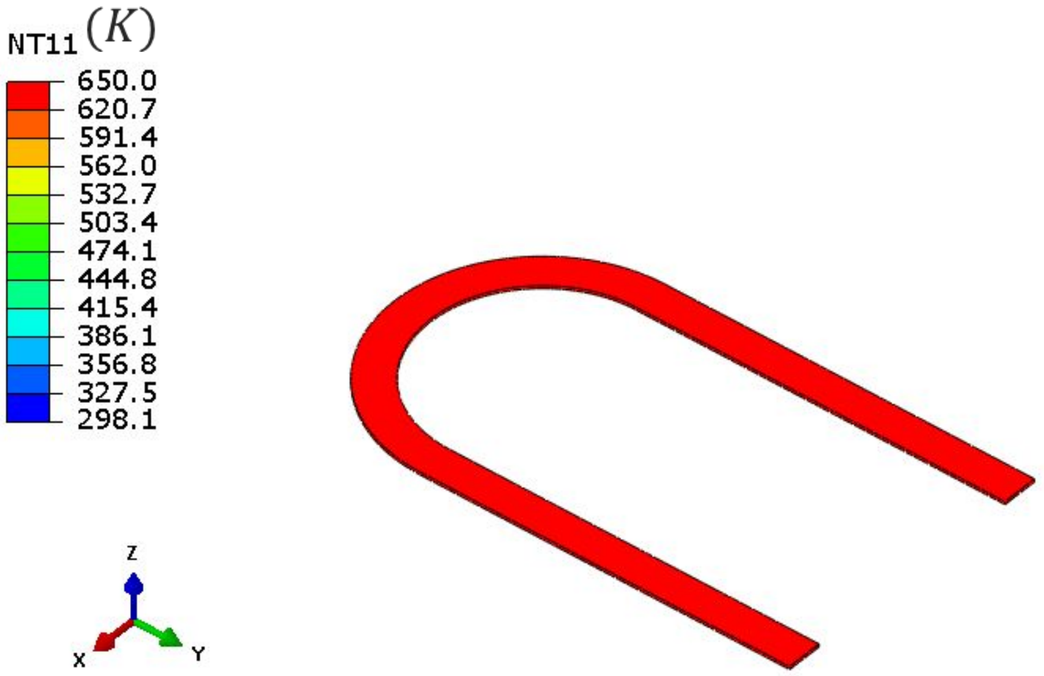
Uneven cooling and contraction between layers causes warping



Finite Element Method (FEM)



Temperature



Limitations of FEM

Requires discretization in space and time → High computational costs

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Is there an alternative?

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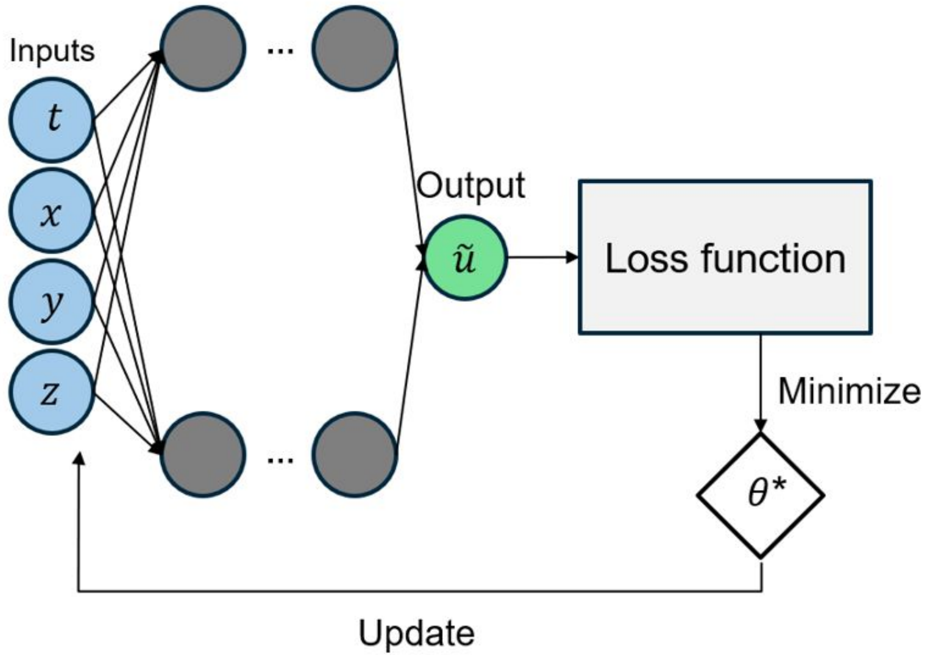
The Core of the Problem: Residual Minimization

- Numerical methods solve PDEs by minimizing the residual
- Residual = PDE(Approximate solution) – Source Term
- To find an approximation solution $\hat{u}$ that minimizes this residual, a common strategy is to:
  - Define a loss function (e.g., MSE)
  - Choose a way to represent $\hat{u}$
  - Optimize the parameter of $\hat{u}$ to minimize the loss function

Neural Networks



- Neural Network (NN) is denoted as $\hat{u}_\theta(\mathrm{X}, t)$
- (X, t) are the input coordinates (space and time)
- θ is the network's learnable parameters
- θ is optimized by minimizing the loss function (predefined based on the PDE residual + boundary/initial conditions)
- The training process tunes θ so that $\hat{u}_\theta$ better satisfies the PDE

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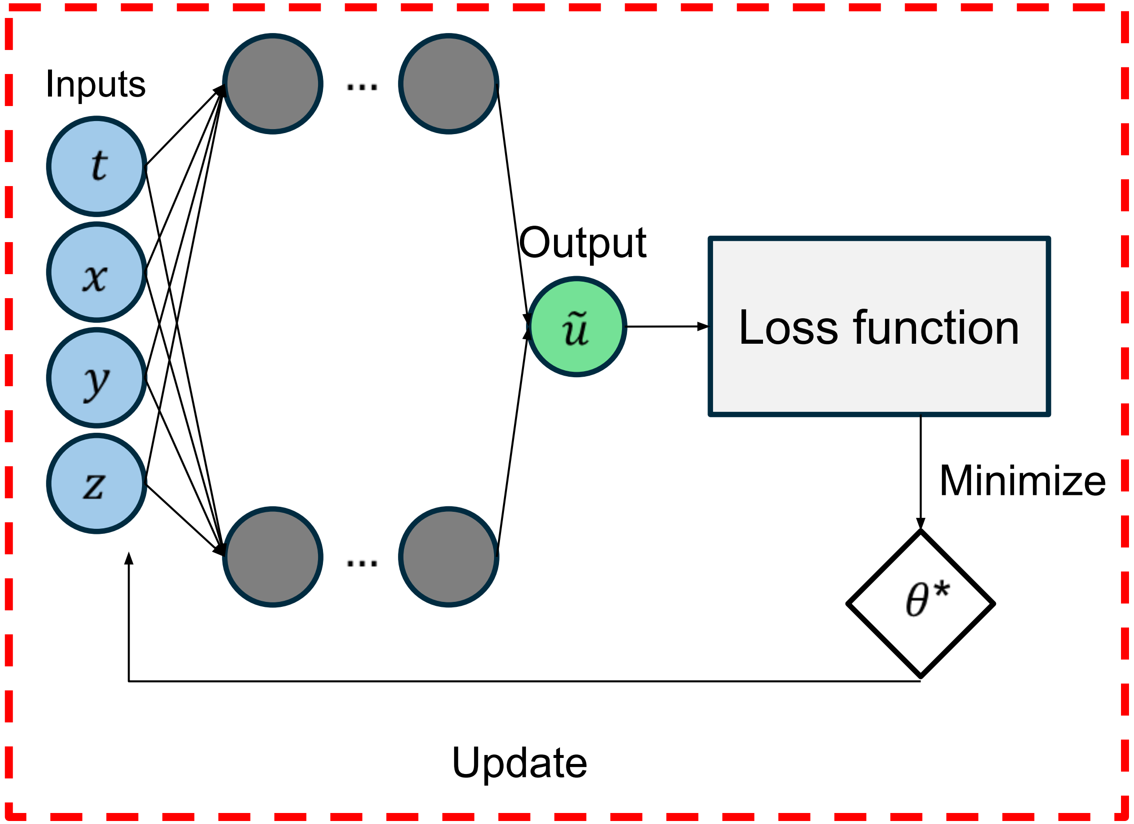
Physics-informed Neural Networks (PINNs)



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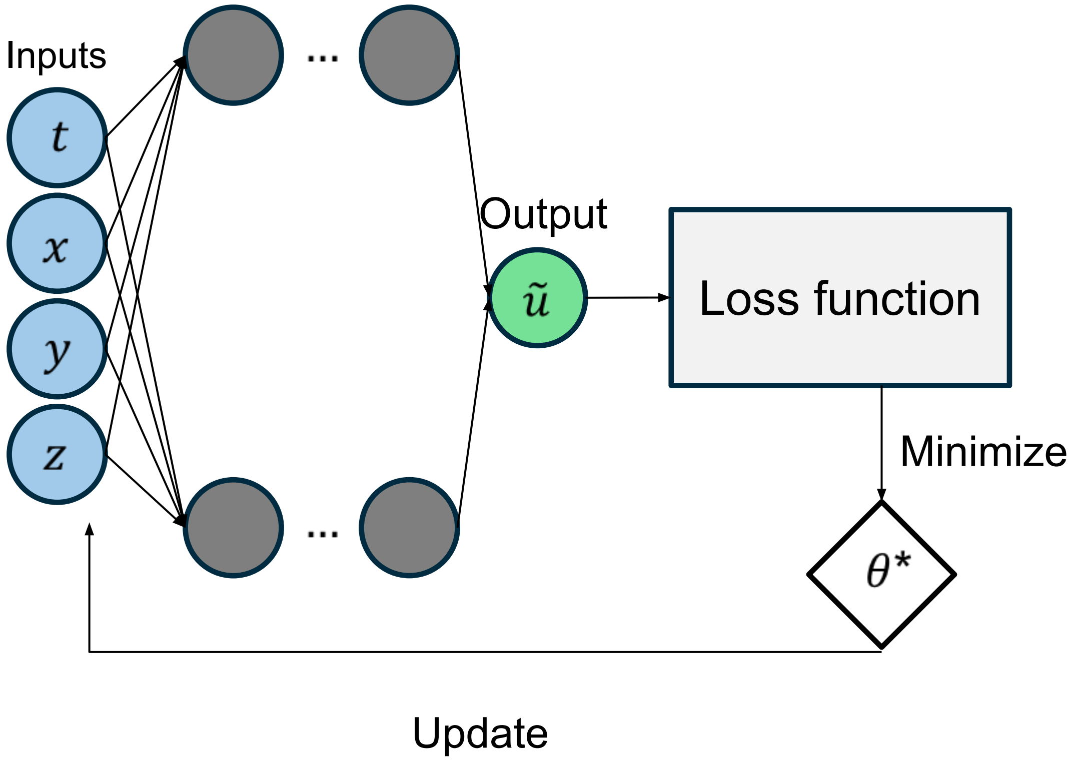

Governing Equation (PDE):

$$\rho C \frac{\partial u}{\partial t} = \nabla \cdot (k(u) \cdot \nabla u)$$

Boundary Condition (BC):

$$k \frac{\partial u}{\partial n} = \underbrace{-h(u - u_\infty)}_{\text{Convection}} - \underbrace{\varepsilon\sigma(u^4 - u_\infty^4)}_{\text{Radiation}}$$

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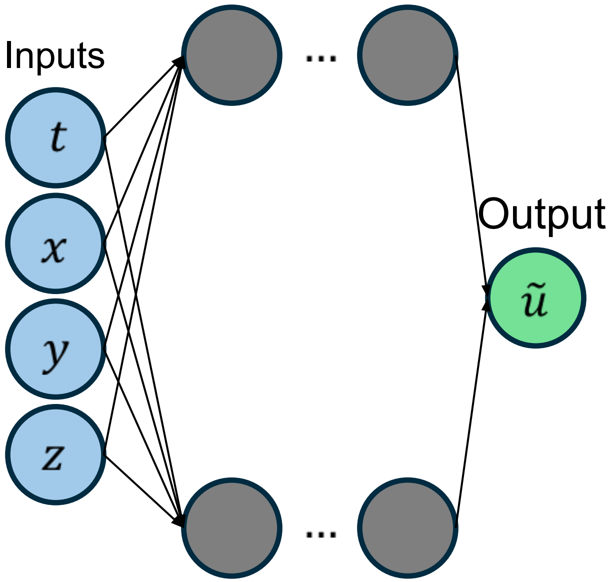

PDE

$$\rho C \frac{\partial \tilde{u}}{\partial t} = \nabla \cdot (k(\tilde{u}) \cdot \nabla \tilde{u})$$

BC

$$k \frac{\partial \tilde{u}}{\partial n} = -h(\tilde{u} - u_{\infty}) - \varepsilon\sigma(\tilde{u}^4 - u_{\infty}^4)$$

Total Loss

PDE residual
+ Boundary Conditions

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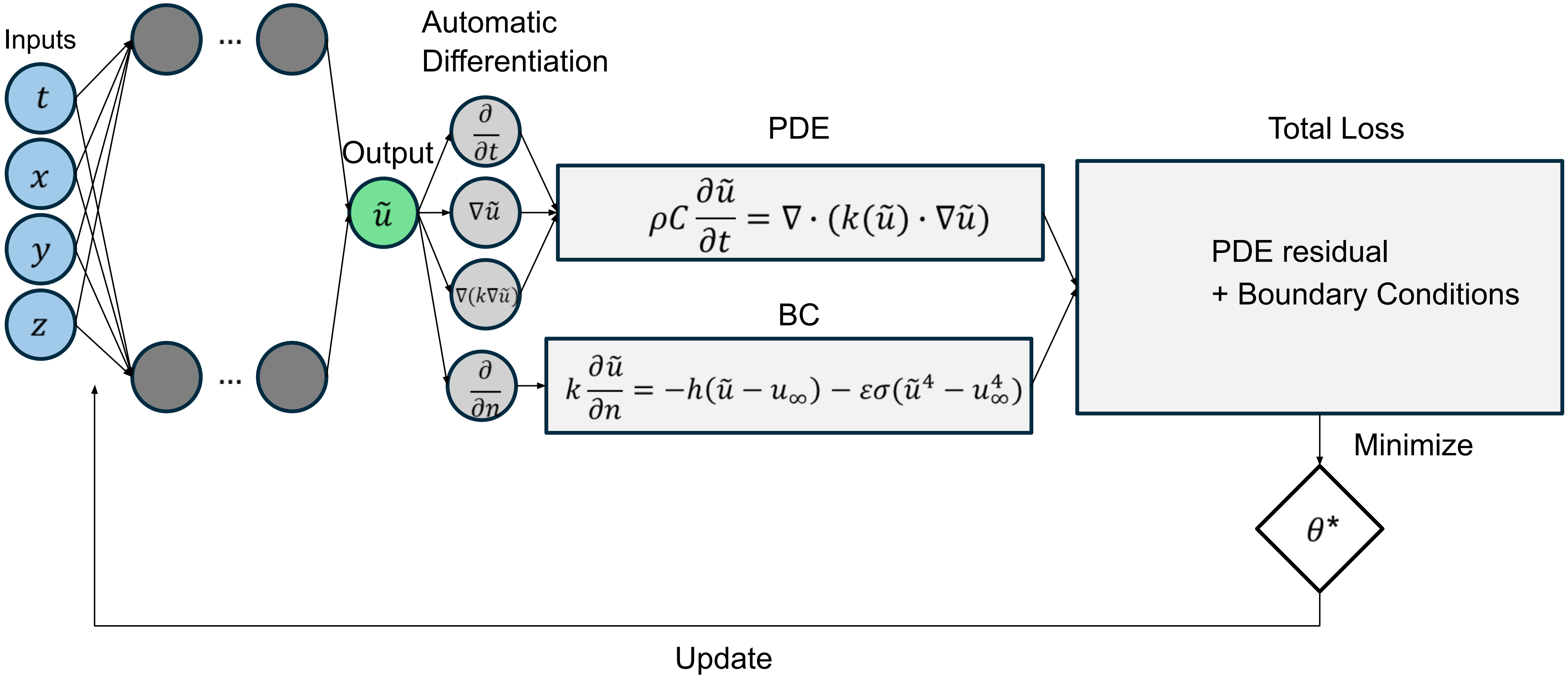
Physics-informed Neural Networks (PINNs)



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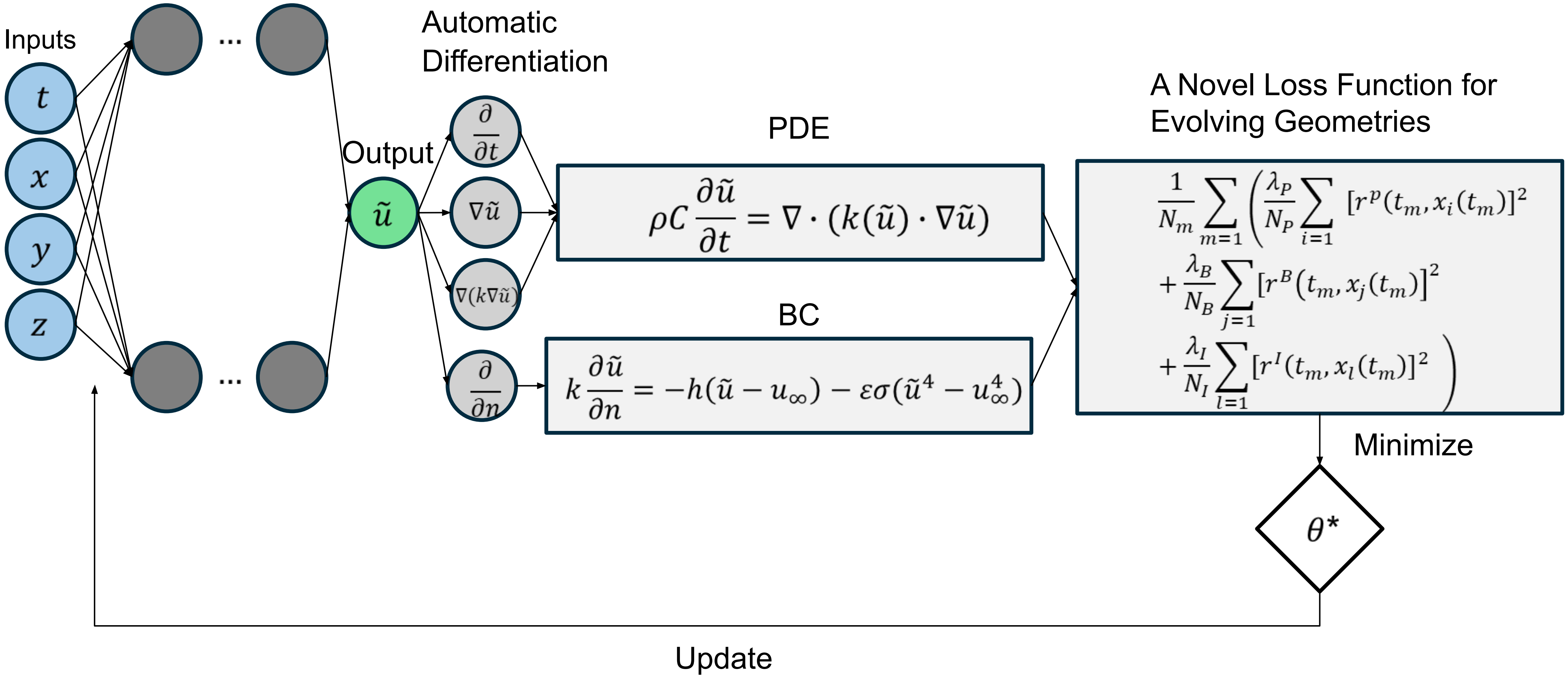
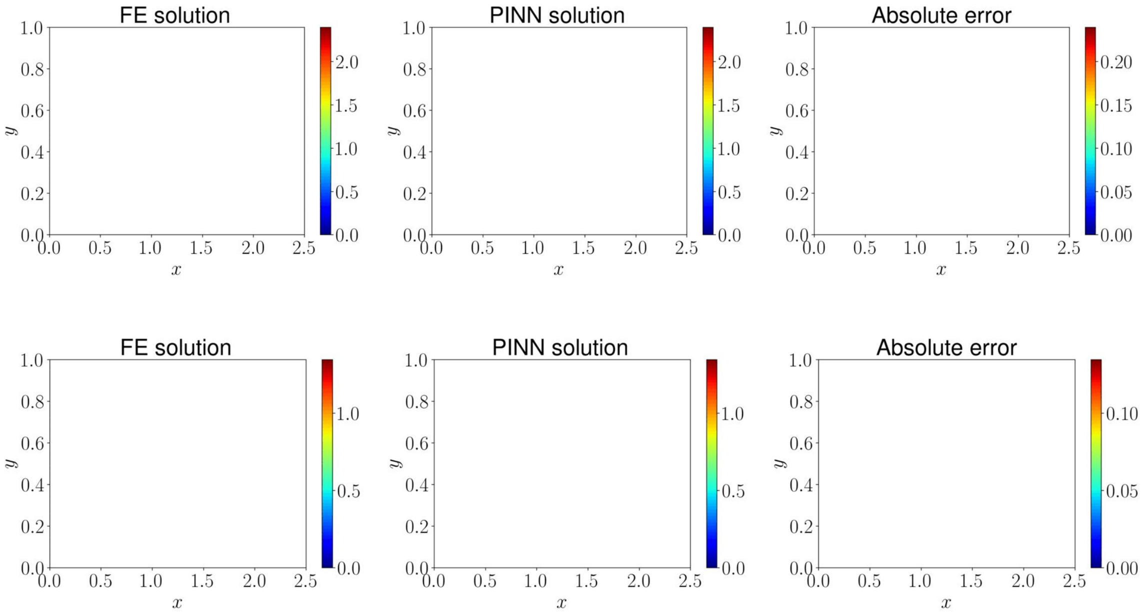


Aim of this work

Demonstrate the feasibility of using **PINNs** for **3D** transient heat transfer problem with **evolving** geometries and **complex boundary conditions**

Prior work

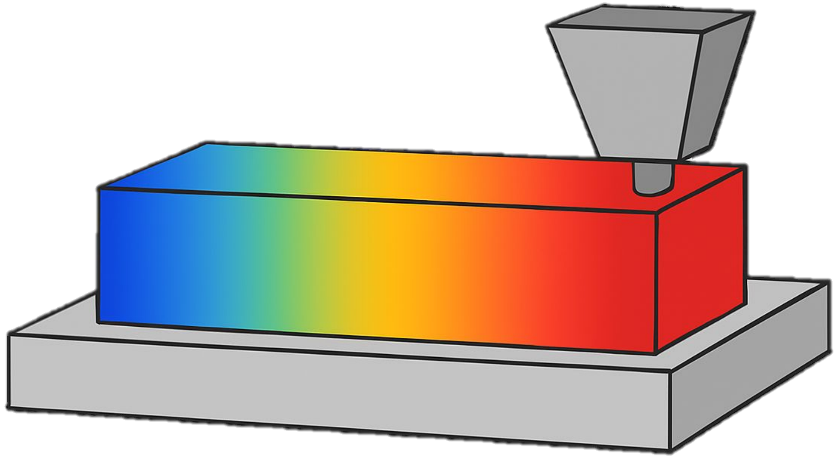
A. J. Thomas et al. (2025) “Causality enforcing parametric heat transfer solvers for evolving geometries in advanced manufacturing” *Computer Methods in Applied Mechanics and Engineering*



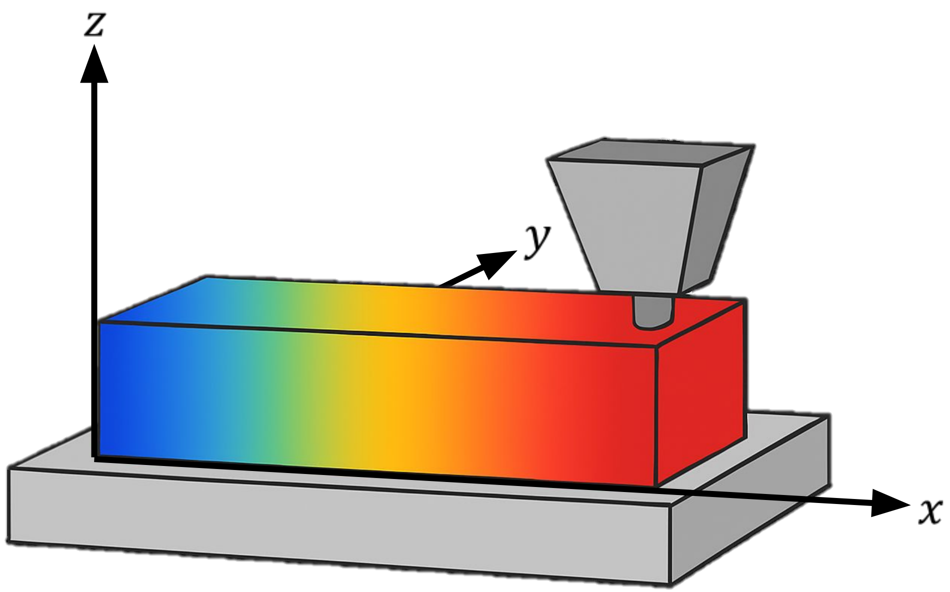
This work builds upon the above work. Specifically,

- **Extend** the formulation from **2D** to **3D** domain
- Incorporate physical complexities such as **radiation** and **temperature-dependent** properties

Methodology



Domain Definition



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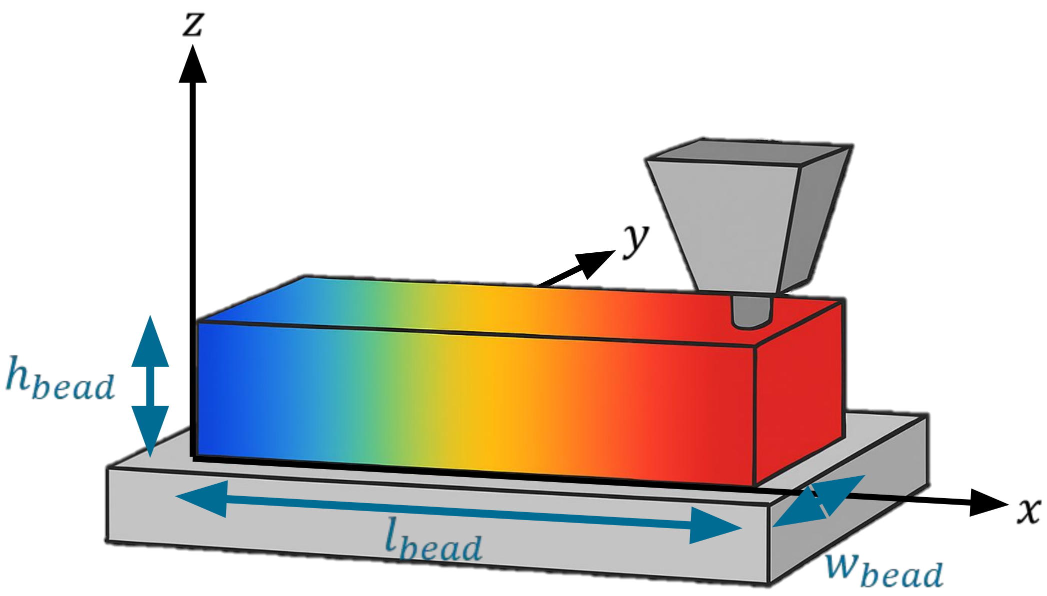

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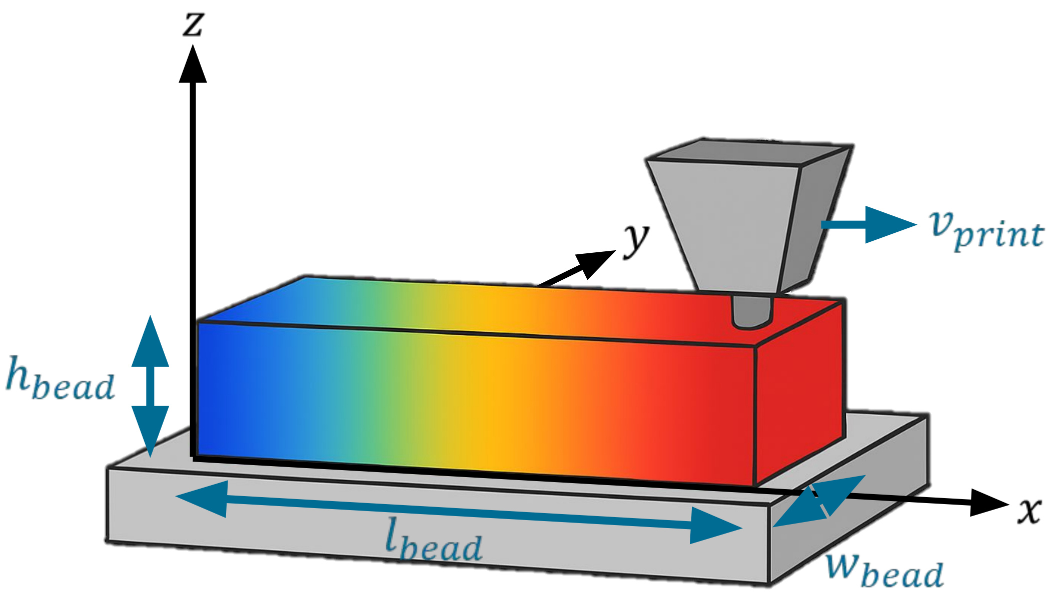
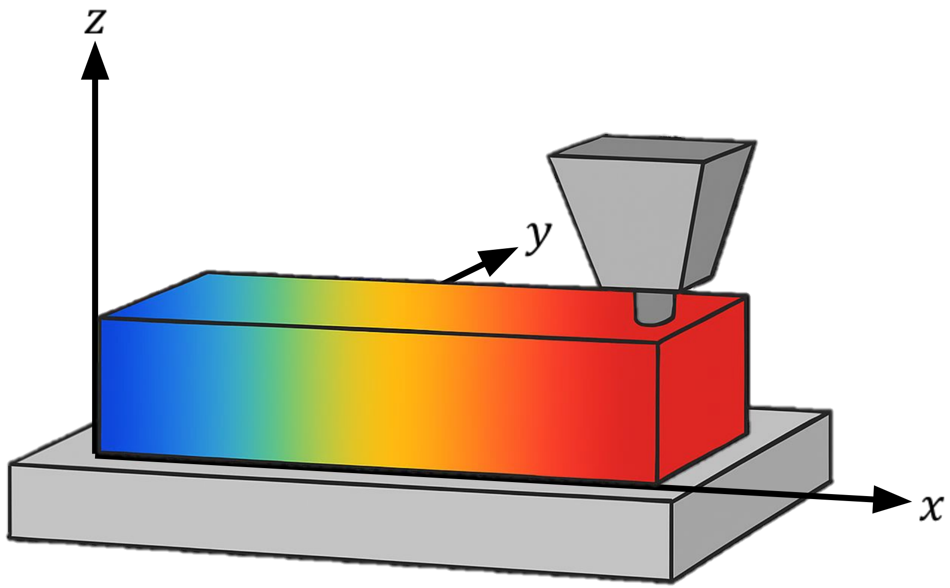
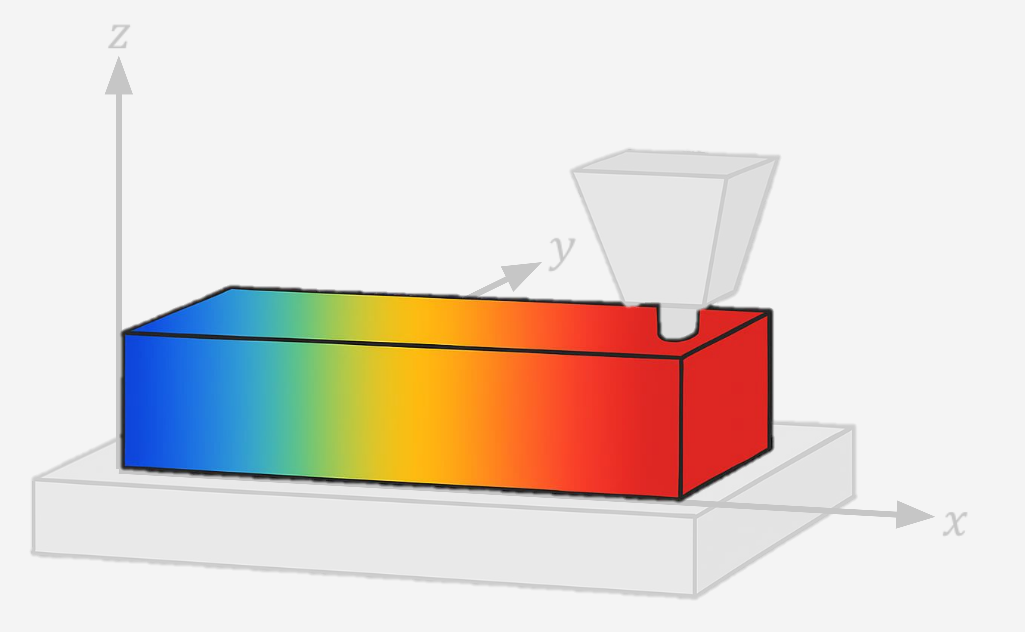


Physical Equations



Physical Equations



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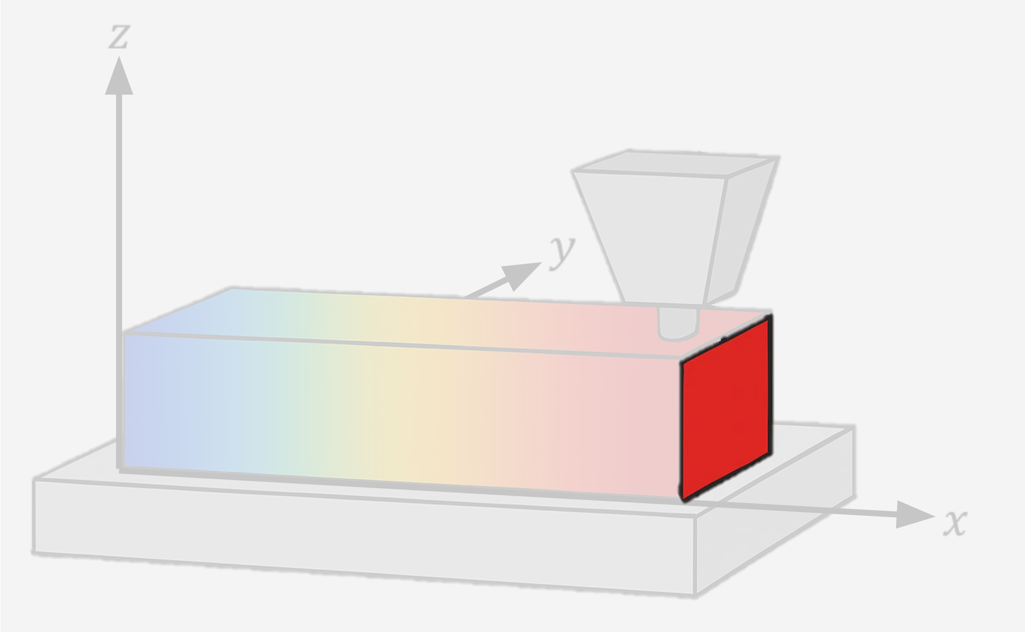
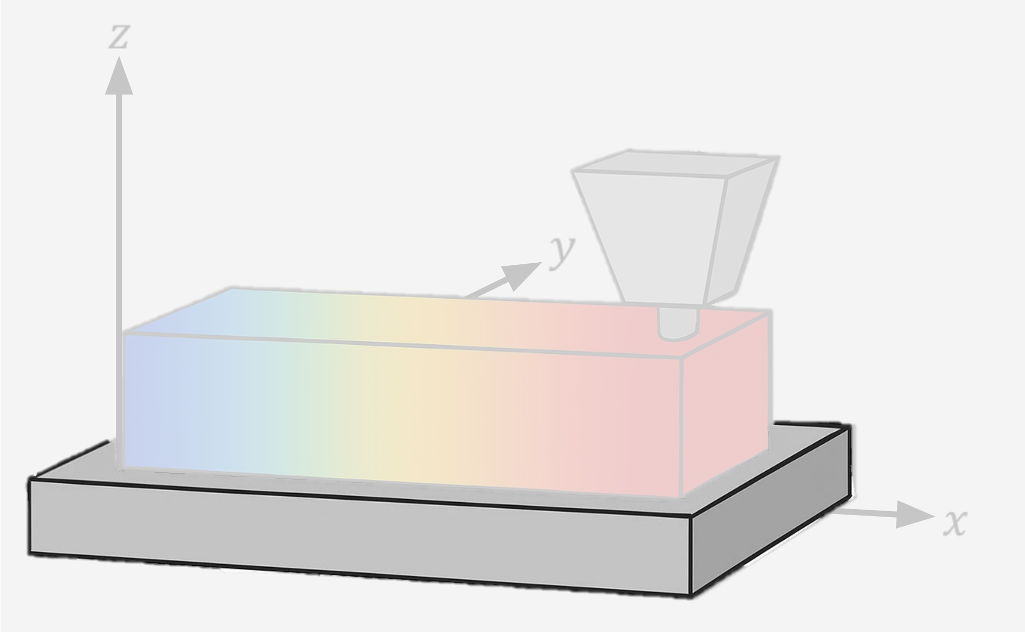


Boundary Conditions (BC):

At deposition front:

$$u(x, y, z, t) = u_{dep}$$

Physical Equations



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At print bed:

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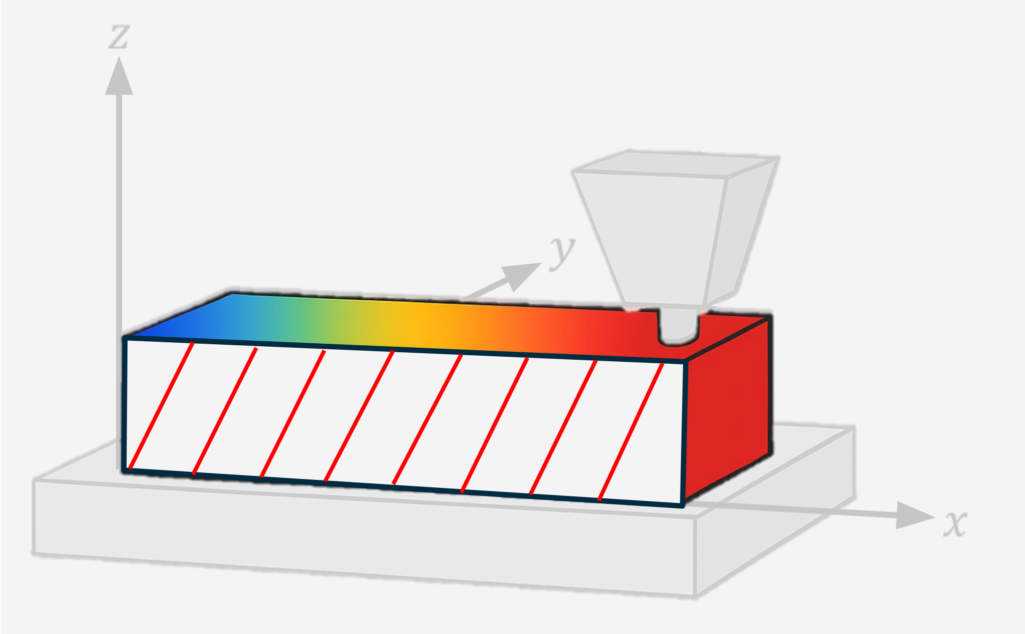
Physical Equations



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Adiabatic (no heat flux):

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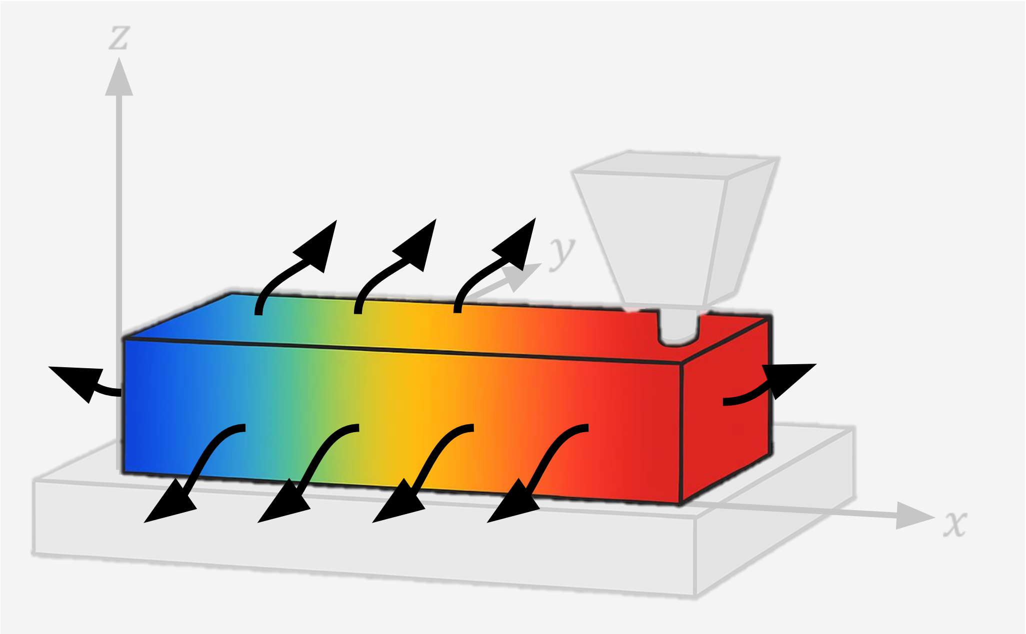

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Convection:

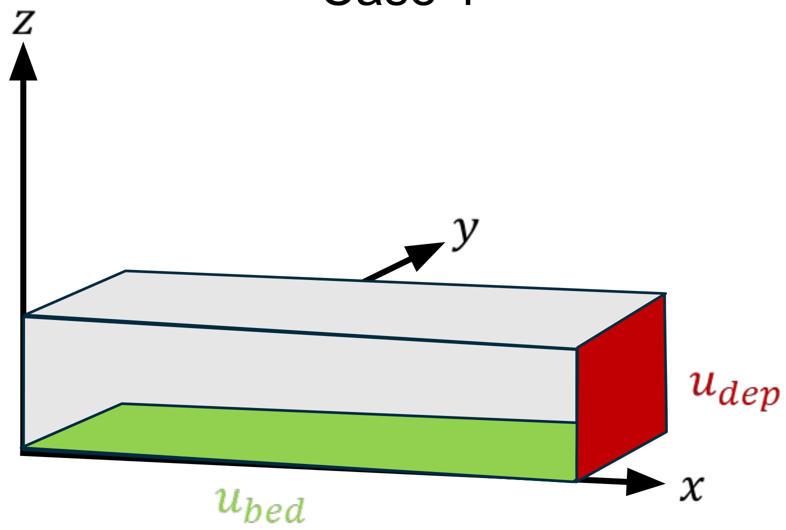
$$k\frac{\partial u}{\partial n} = -h(u - u_{\infty})$$

Radiation:

$$k\frac{\partial u}{\partial n} = -\varepsilon\sigma(u^4 - u_{\infty}^4)$$

Case Study:
Evolving Geometries with Increasing Complexity

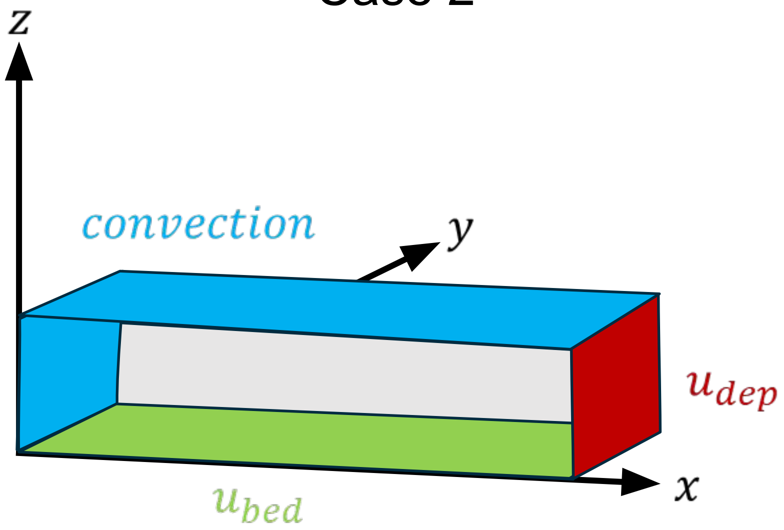
Case 1



Conditions enforced:

1. Constant deposition surface
2. Evolving bed surface

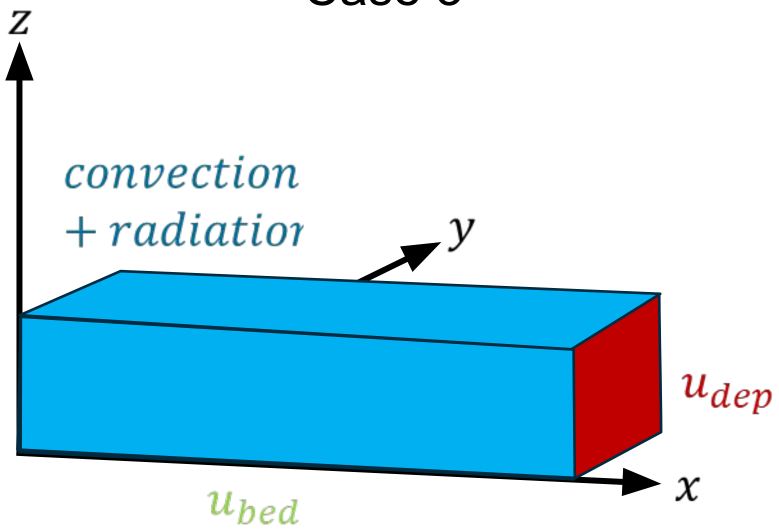
Case 2



Conditions enforced:

1. Constant deposition surface
2. Evolving bed surface
3. Constant and evolving surfaces with convection

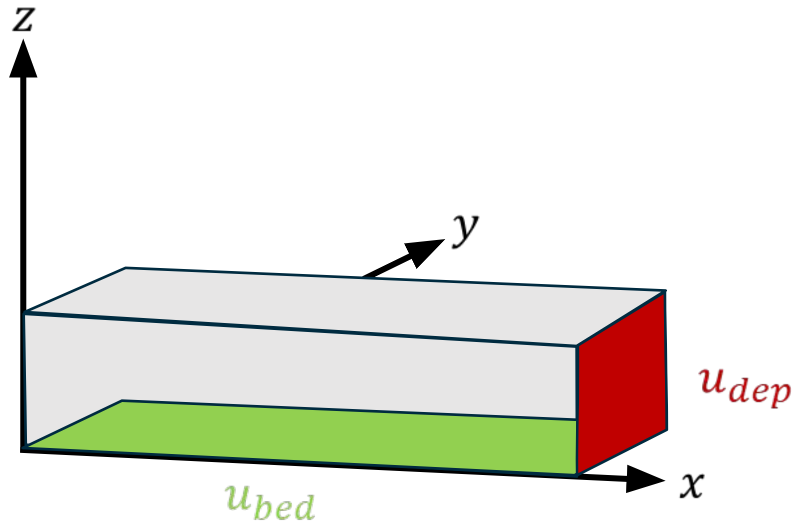
Case 3



Conditions enforced:

1. Constant deposition surface
2. Evolving bed surface
3. Constant and more evolving surfaces with convection + radiation

Case 1



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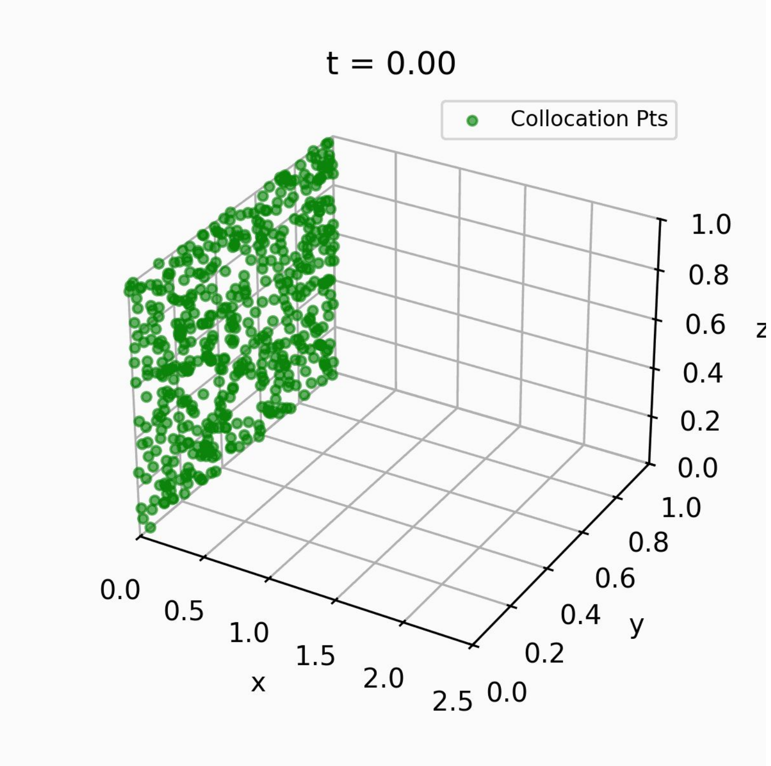

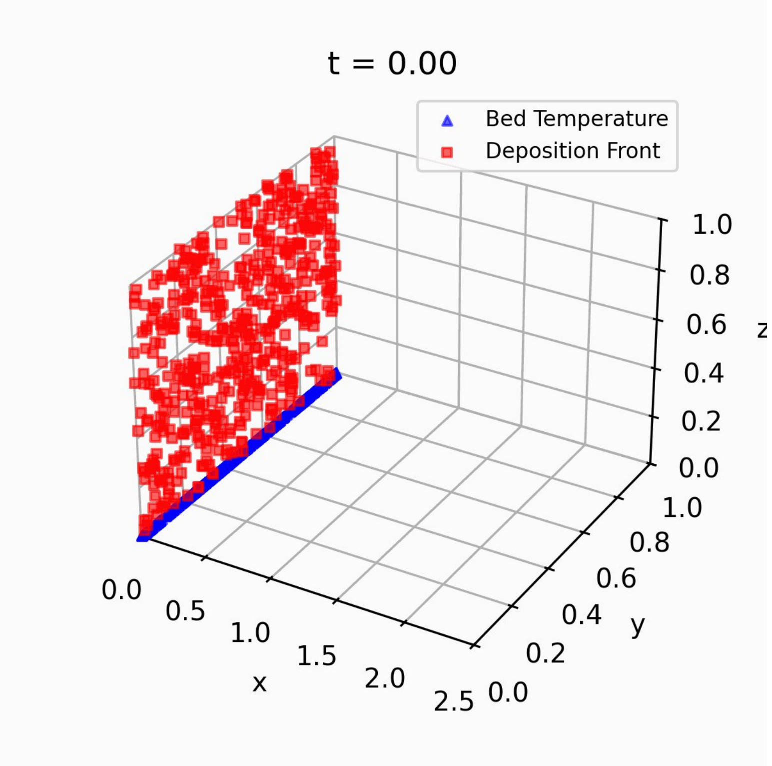

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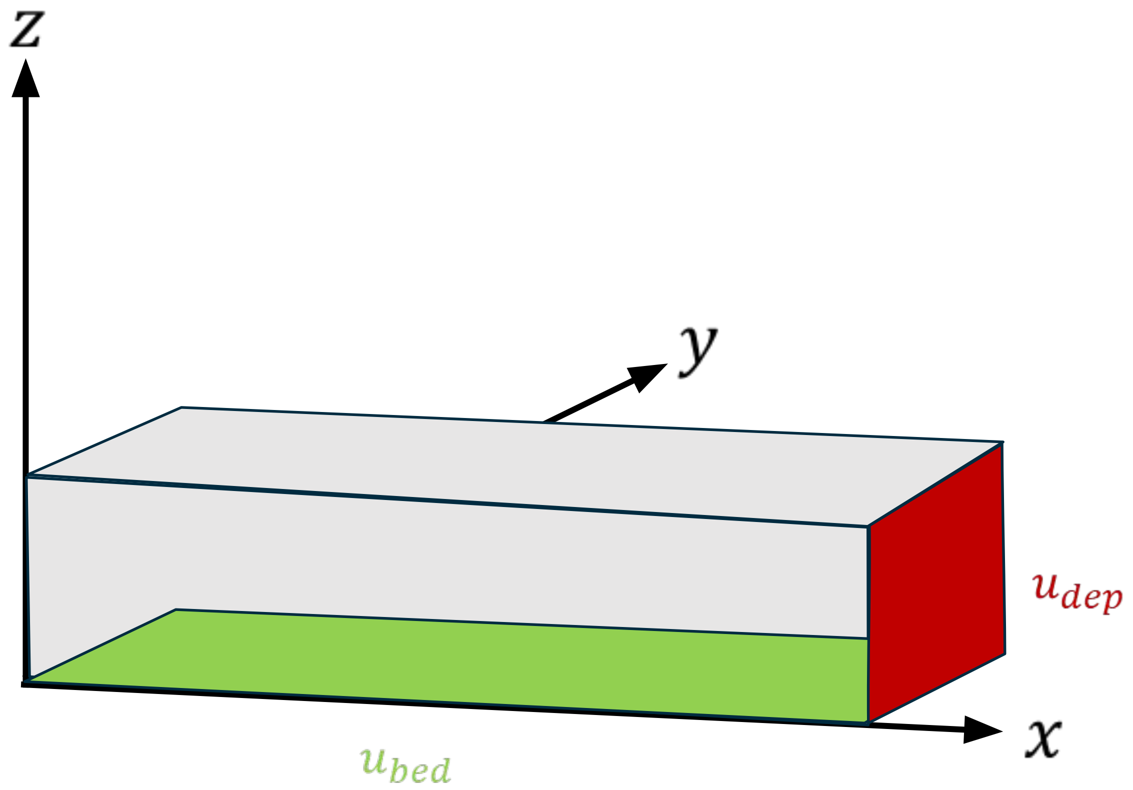
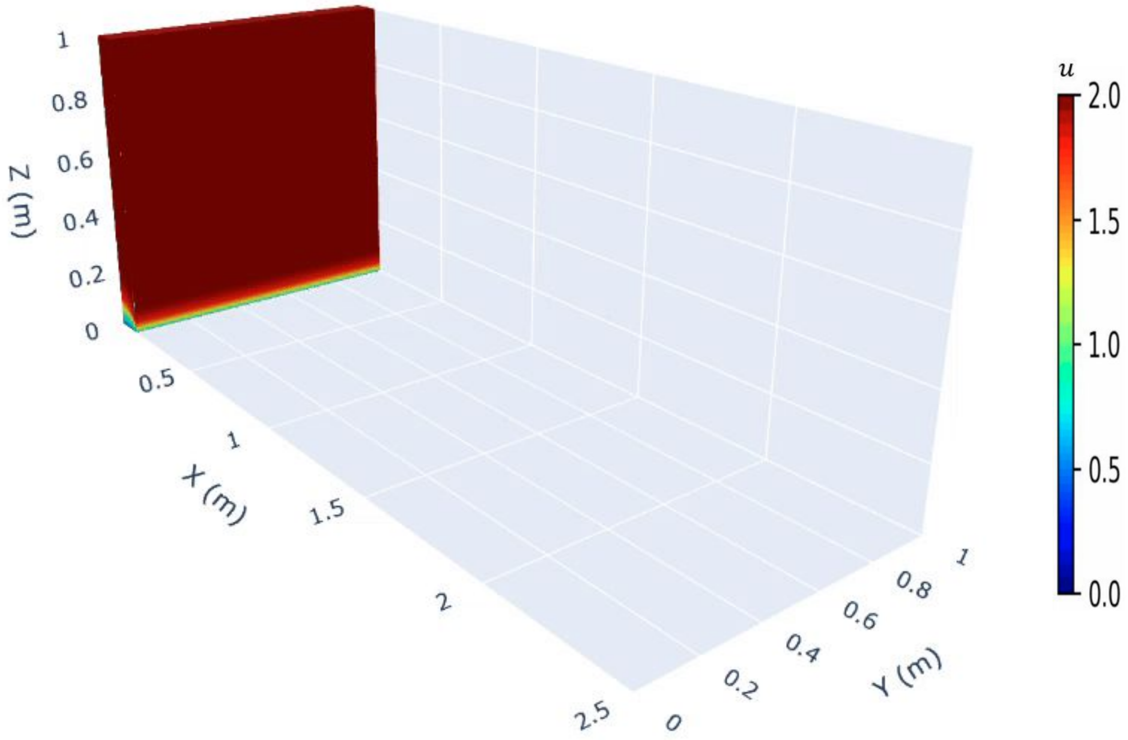
Visual Result: Case 1





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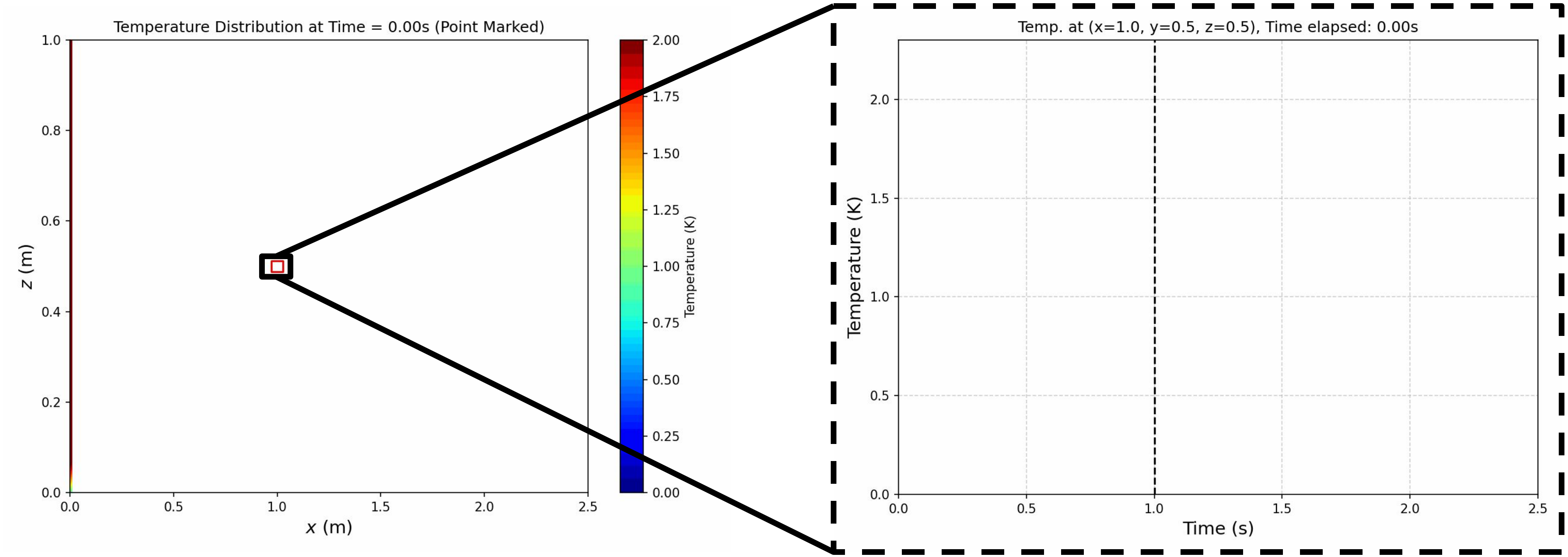
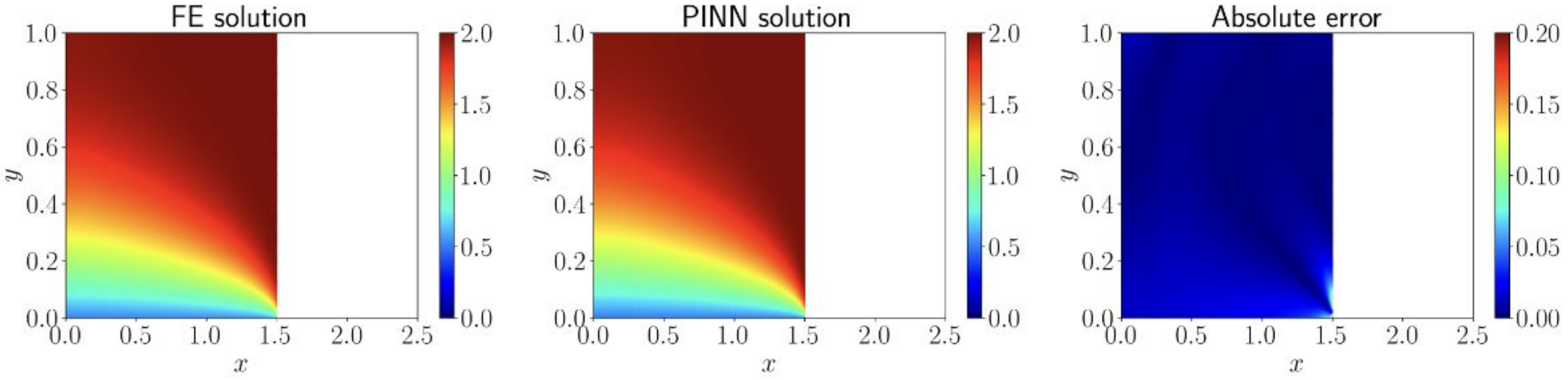
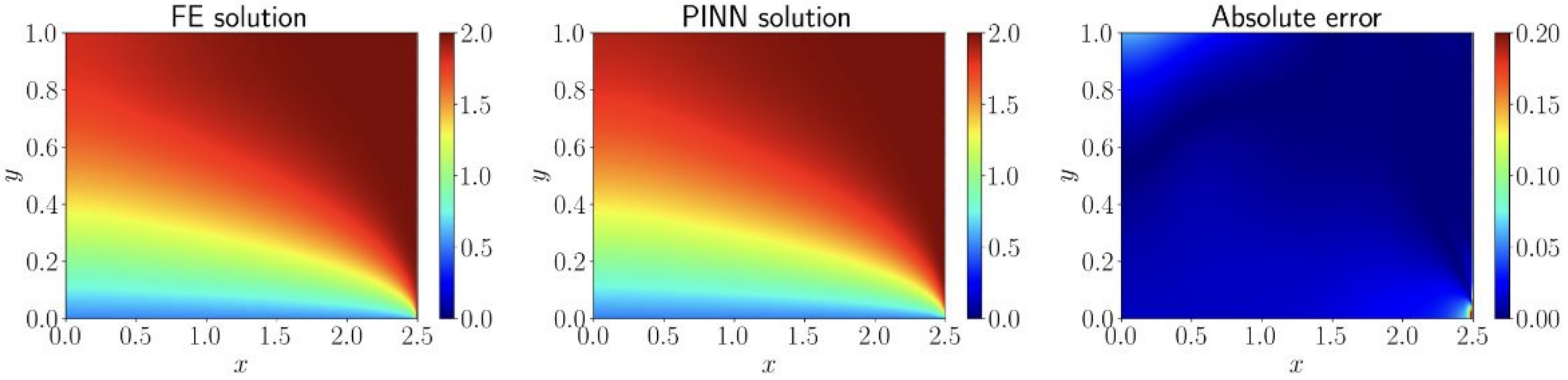


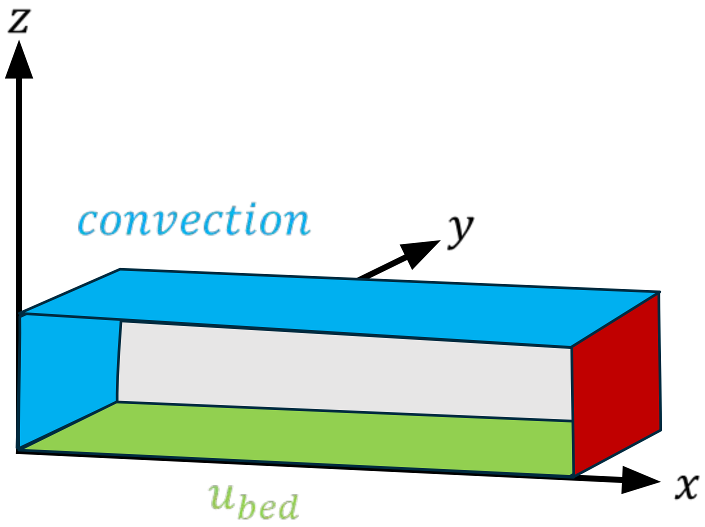
Comparison with FEM: Case 1



(c) At $t = 1.5$



Case 2



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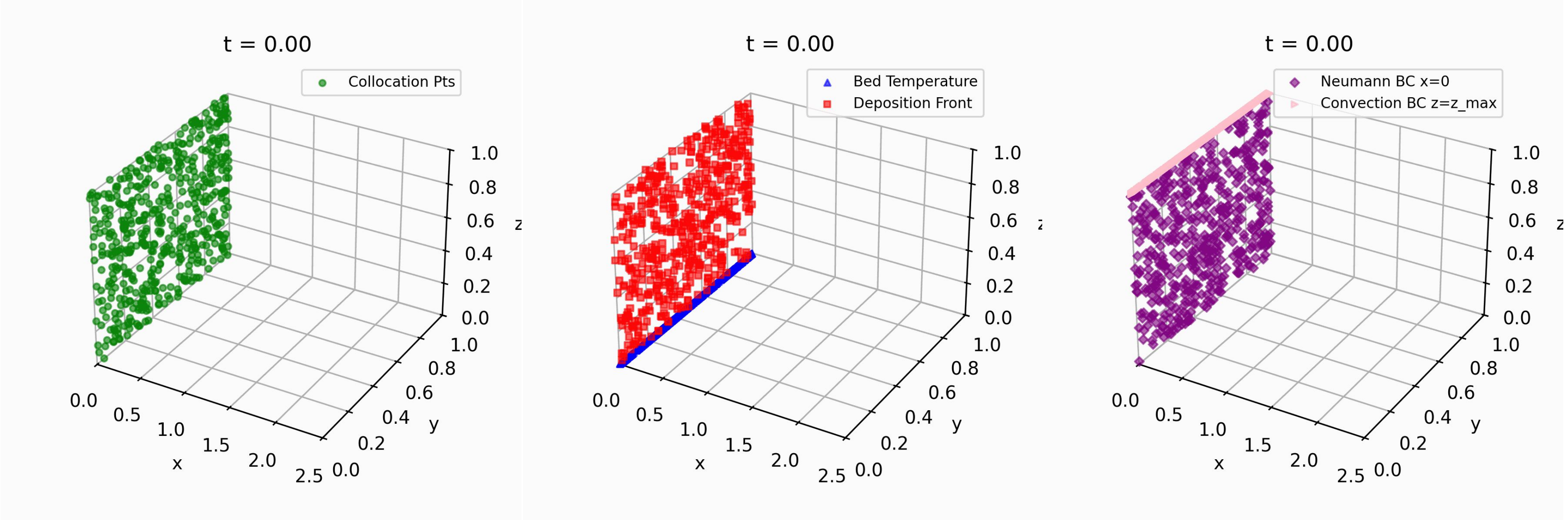
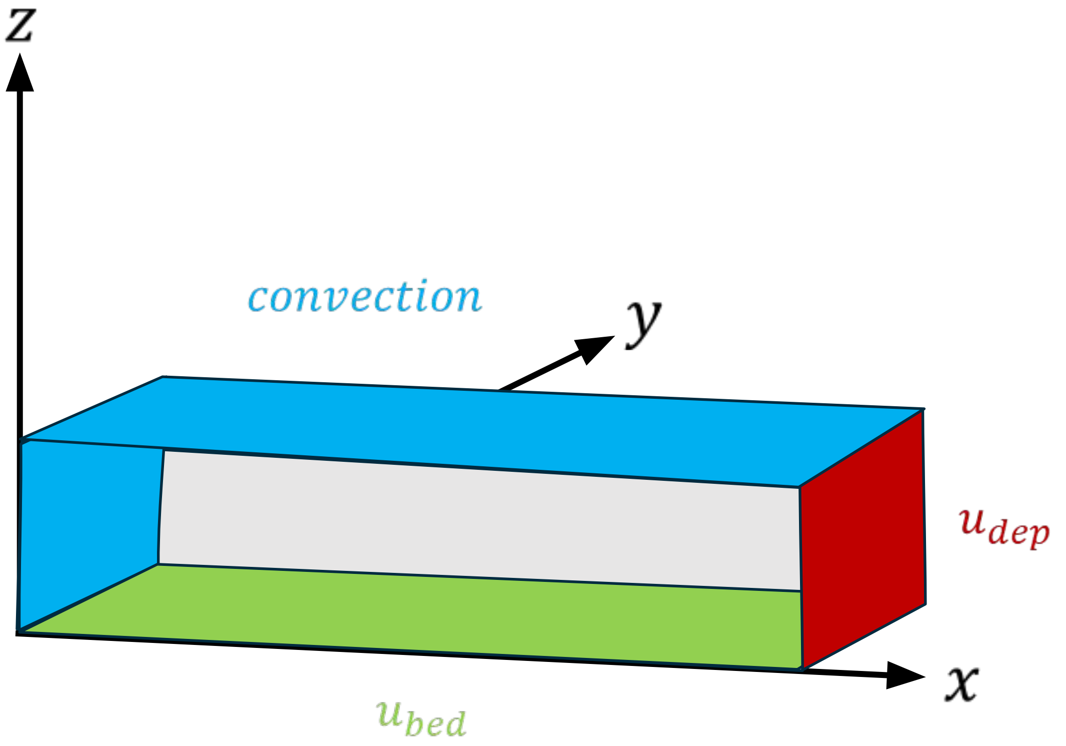
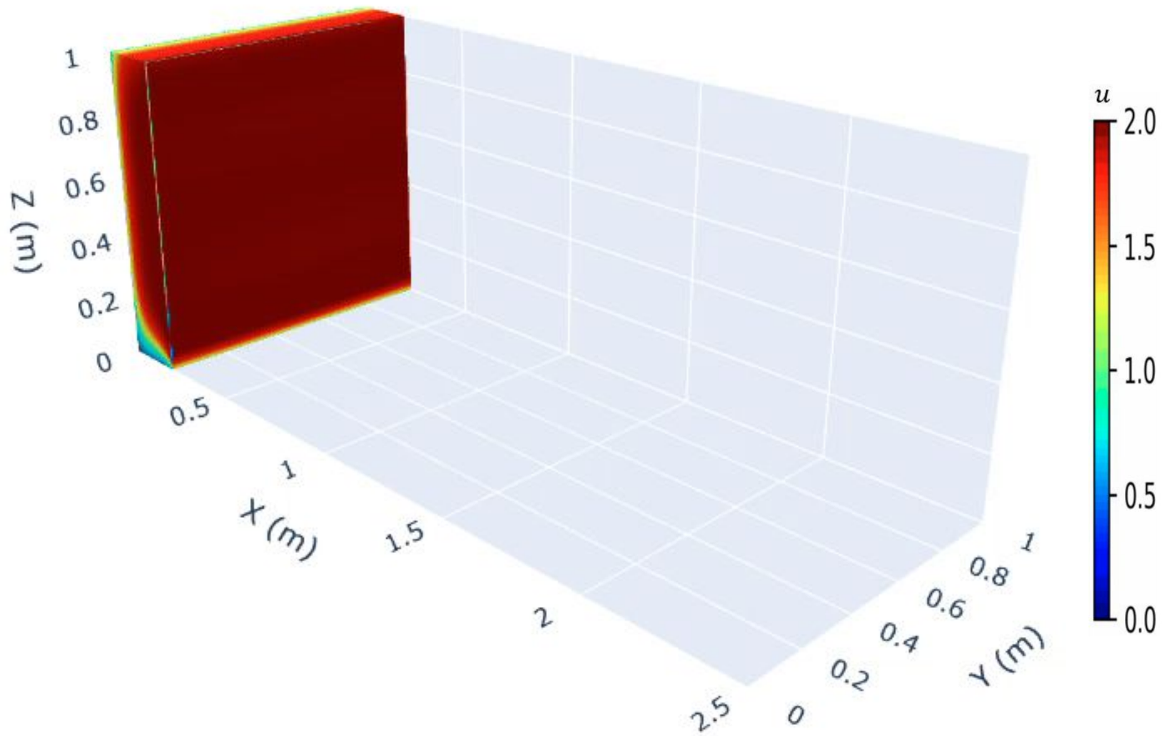
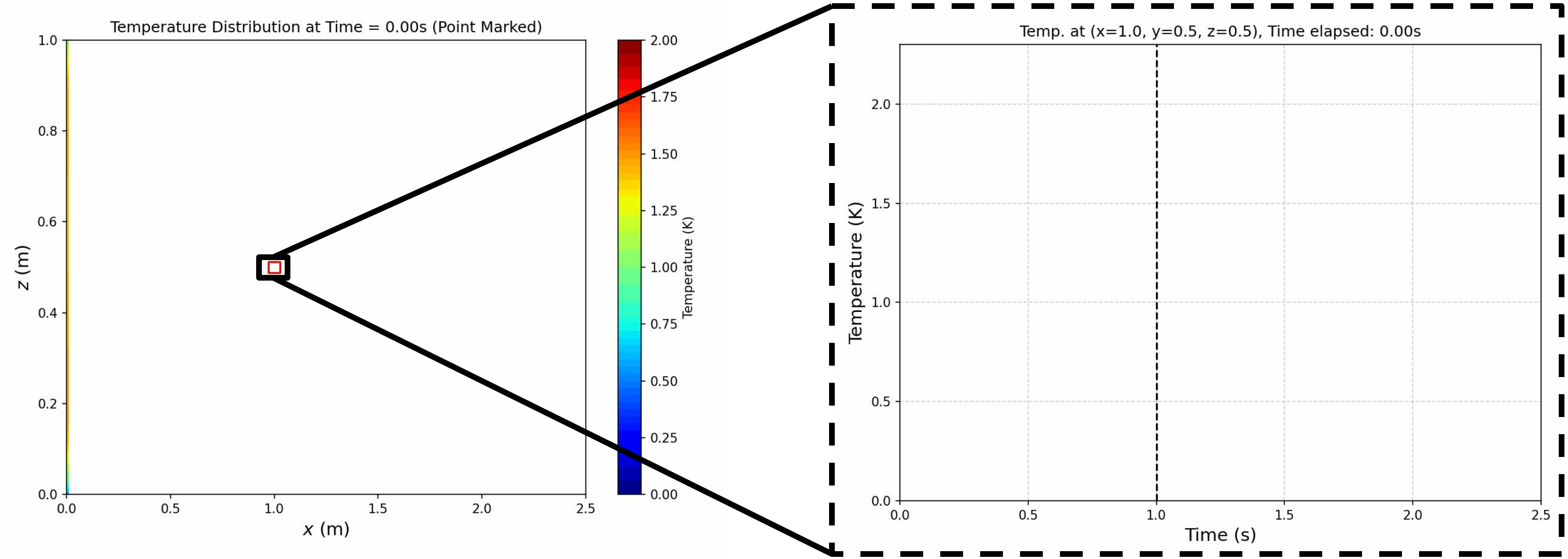


Visual Result: Case 2





Visual Result: Case 2



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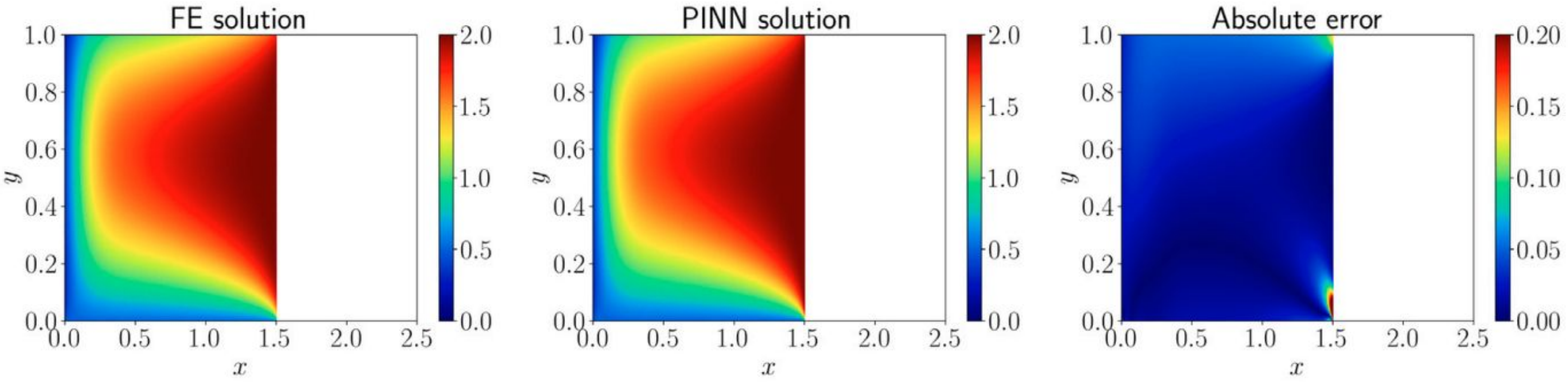
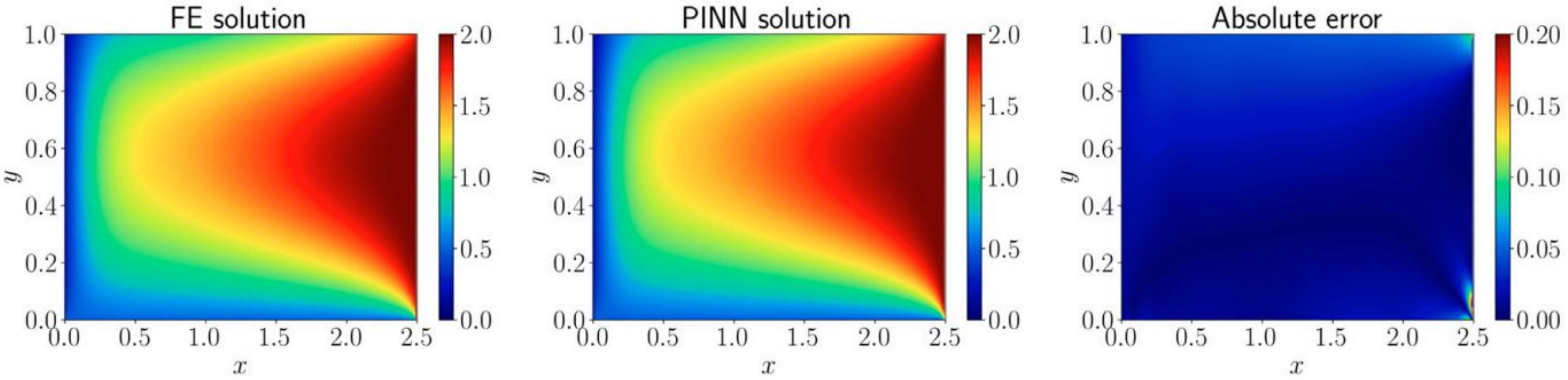
Comparison with FEM: Case 2



(b) At $t = 1.5$



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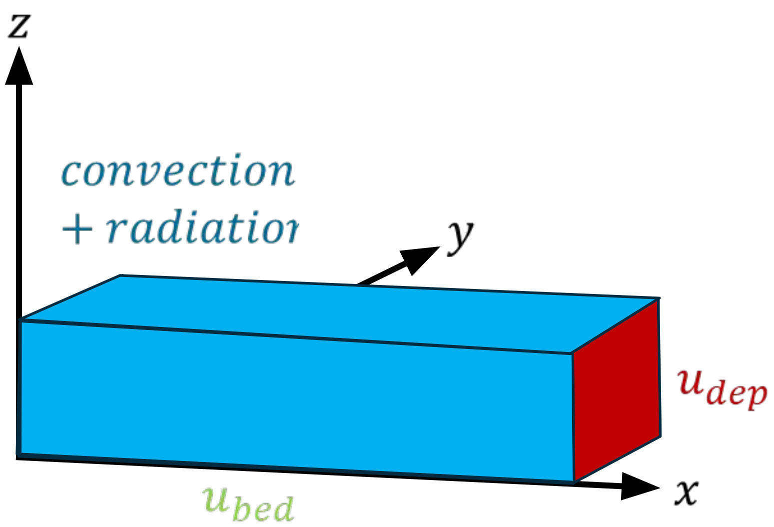
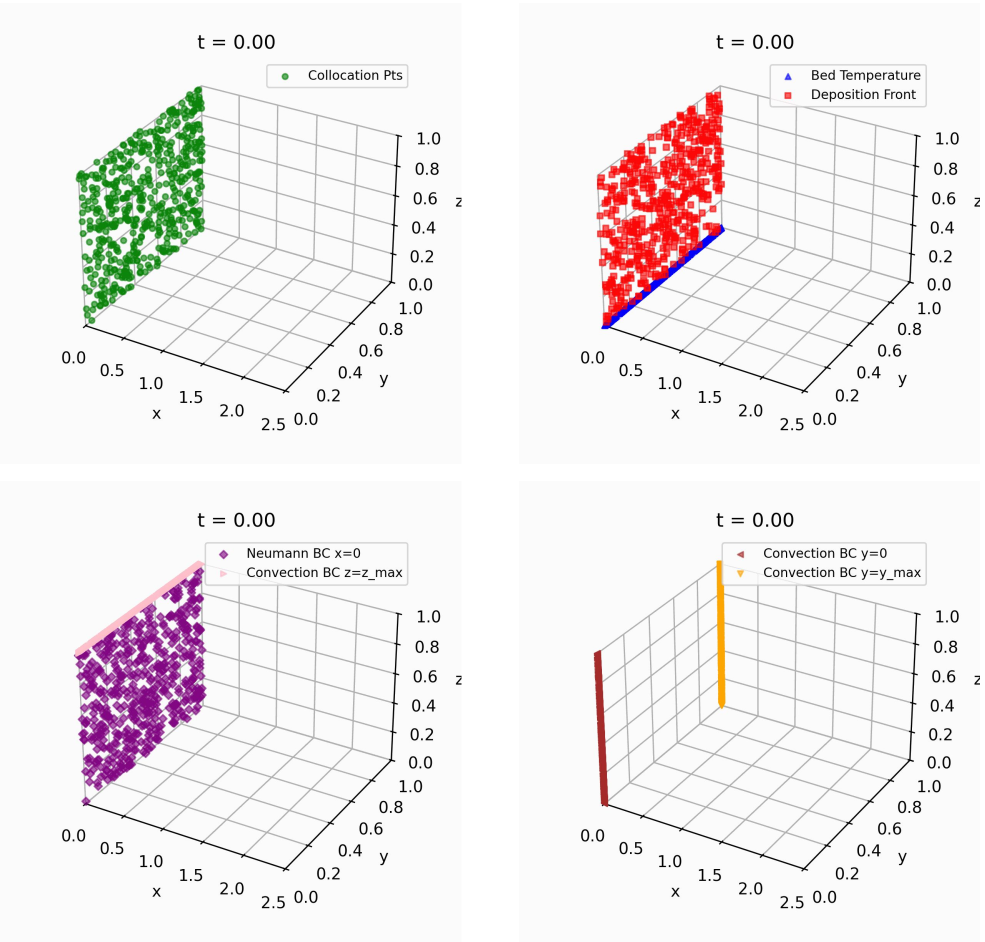
Case 3





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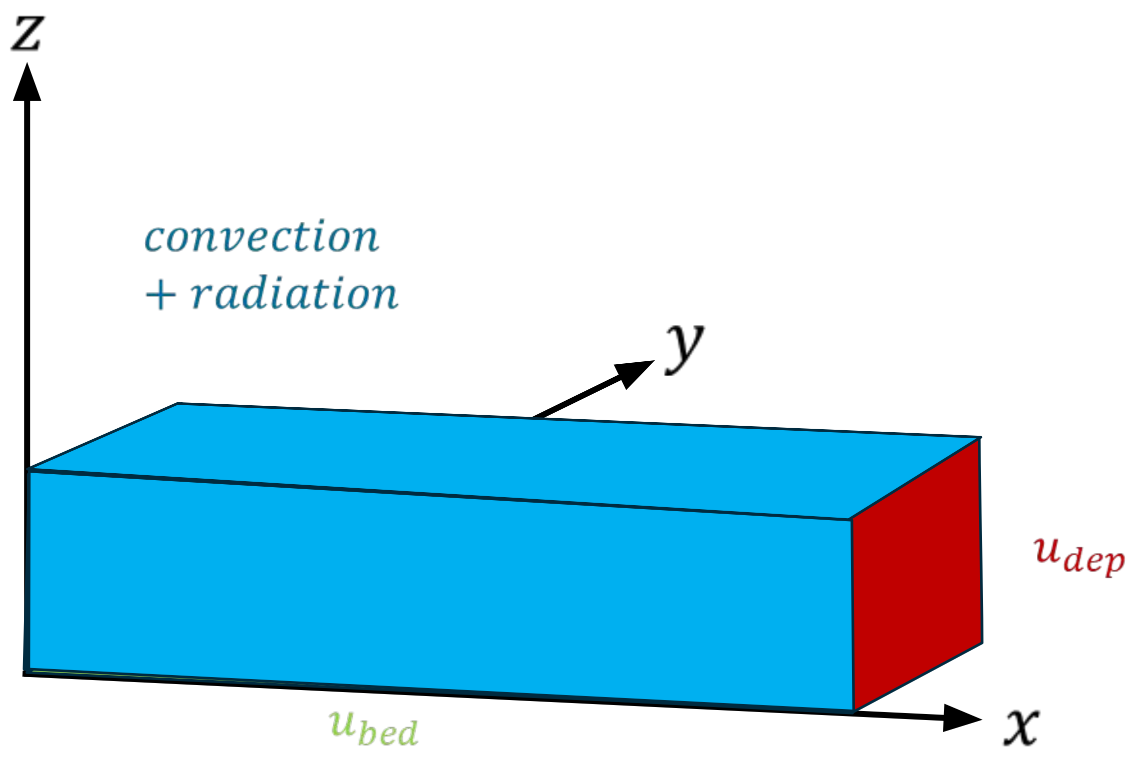

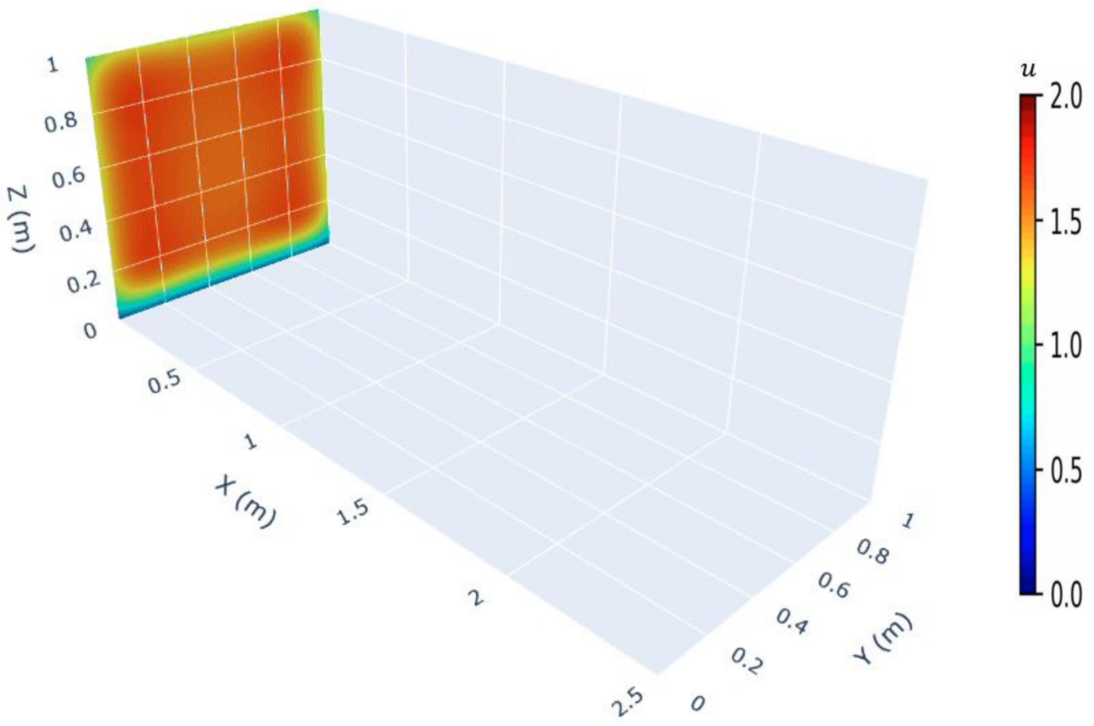

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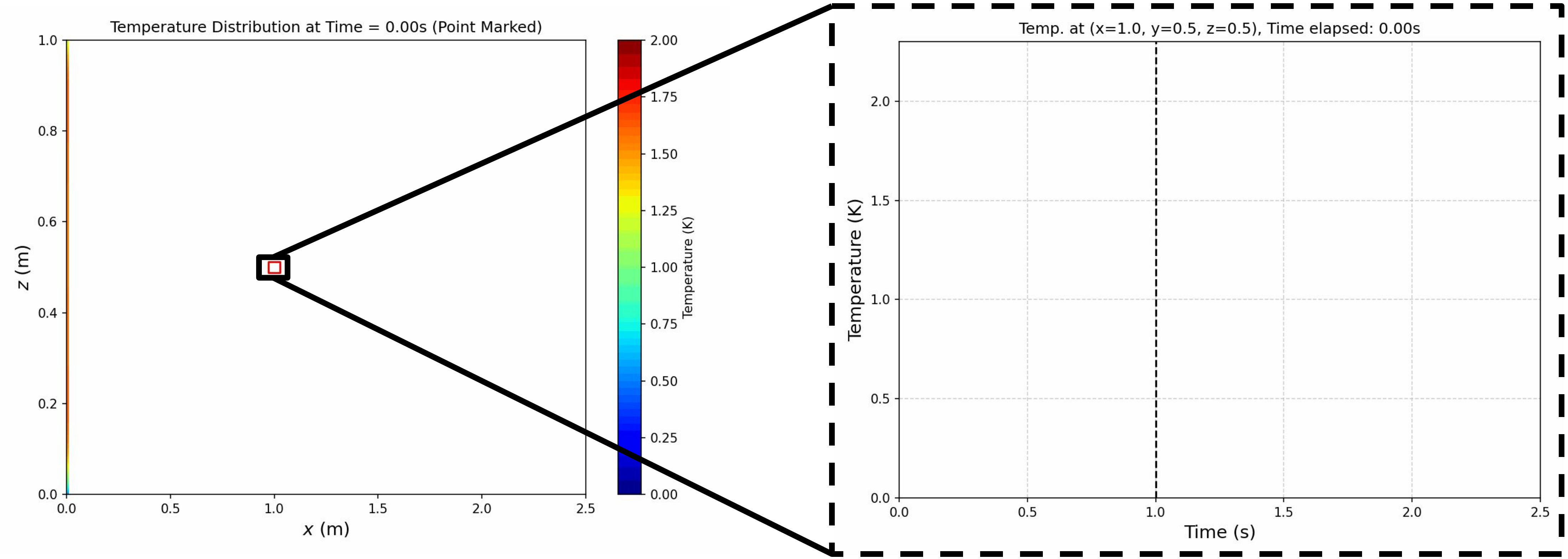
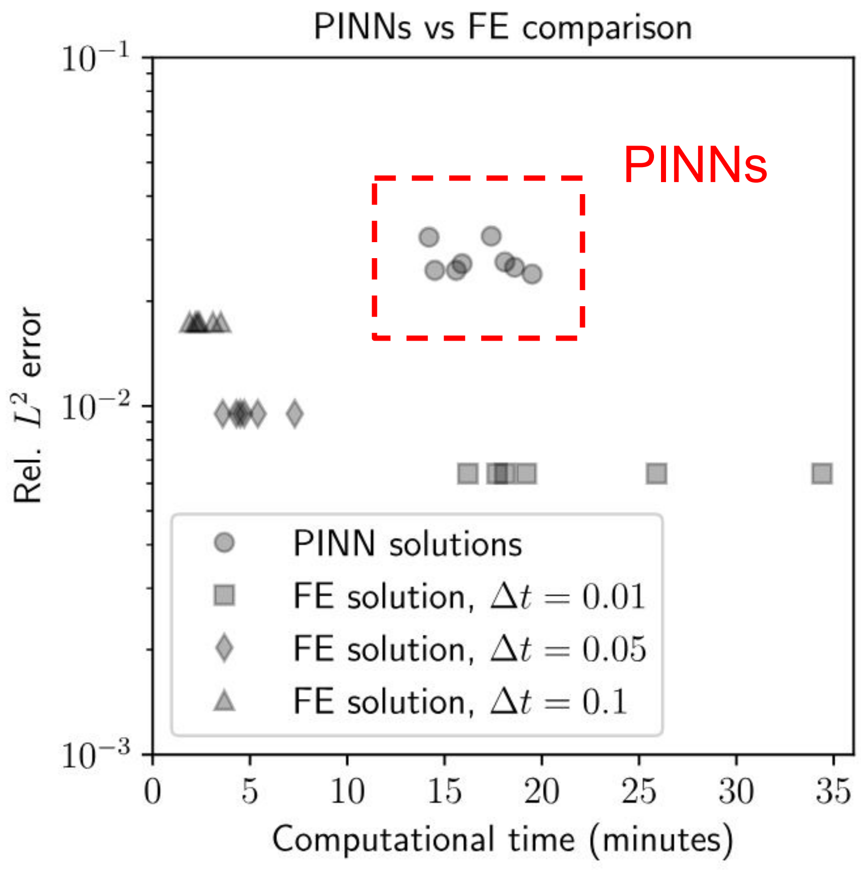


Computational Time



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Parametric Problems

- Material properties or process conditions have inherent variability
  - e.g. Deposition temperature, Bed temperature, Convection coefficient, Thermal conductivity… etc.
- Aim is to see how the temperature field changes across a range of these parameters

Parametric PINNs

- A single PINNs can learn the solution across a range of these parameters
- The parameters are additional inputs to the NN

New loss function for parametric problems:

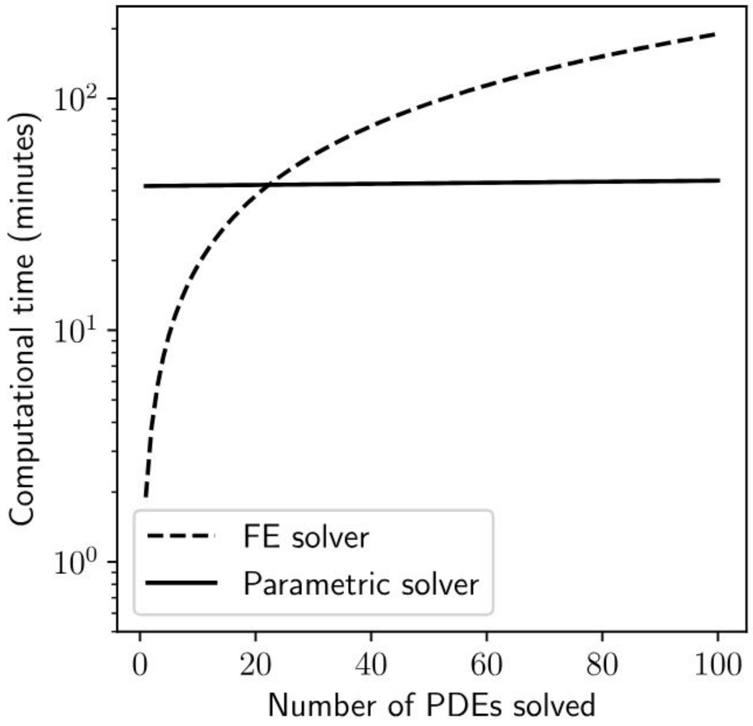
$$l_e = \int d\xi \int_0^T dt \; l(t, x(t), \xi_v ; \theta)$$

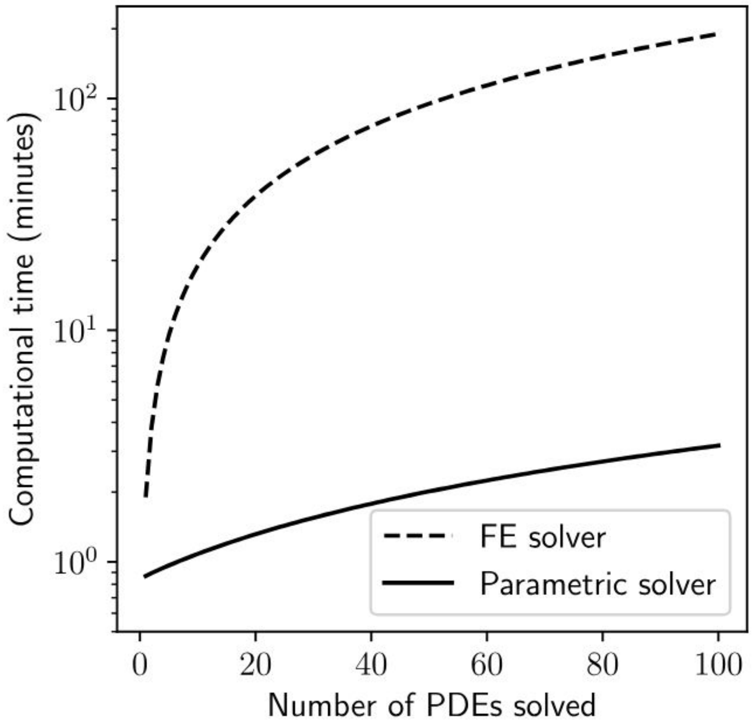
Temperature field is parametrized as:

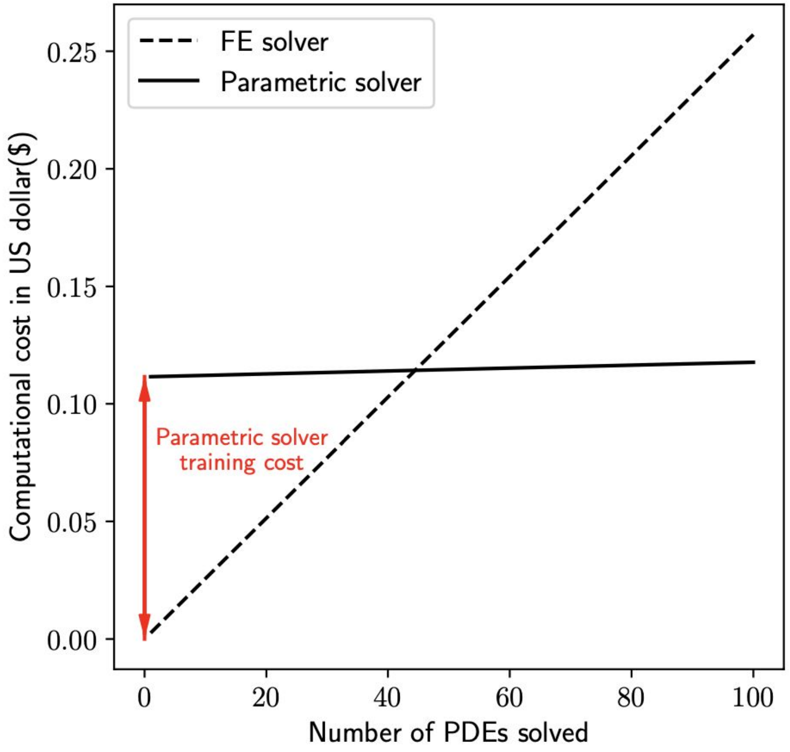
$$u_\theta(\tilde{t}, \tilde{\mathbf{x}}, \tilde{\xi}; \theta) = \sum_{i=1}^{g} \underbrace{\psi_i(\tilde{\xi}; \theta)}_{\text{branch}} \underbrace{\phi_i(\tilde{t}, \tilde{\mathbf{x}}; \theta)}_{\text{trunk}}$$

Once trained, predicting the solution for any new set of parameters is almost immediate!

Parametric Solver







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Conclusion

- PINNs offer a **mesh-free** framework for **3D** heat transfer problem with **evolving geometries** and **complex boundary conditions**

- FEM is **faster** and **more accurate** for single forward problems

- PINNs have potential for **parametric** problems

Future Work

- Extension to arbitrary geometries
- Extension to multi-layer deposition

We aim to build surrogate models without having to run FEM

Thank you!

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