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# Physics-Informed Neural Networks for Multiphysics Simulations: Application to Coupled Electromagnetic-Thermal Modeling


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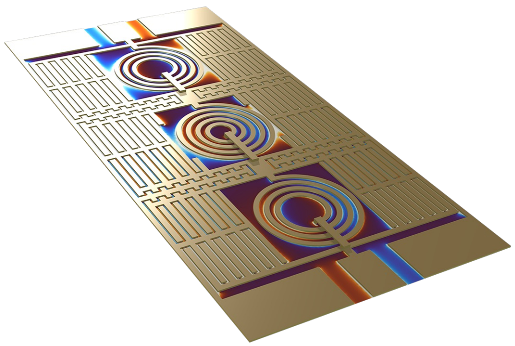
# Outline

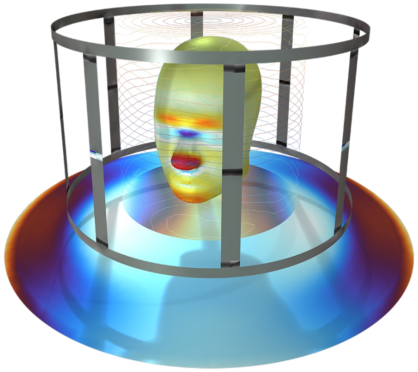
- Background and motivation
- Review of electromagnetic-thermal simulations
- Physics-informed neural networks for electromagnetic-thermal simulations
- Numerical Results
- Conclusions

## Challenges of multi-physics simulation

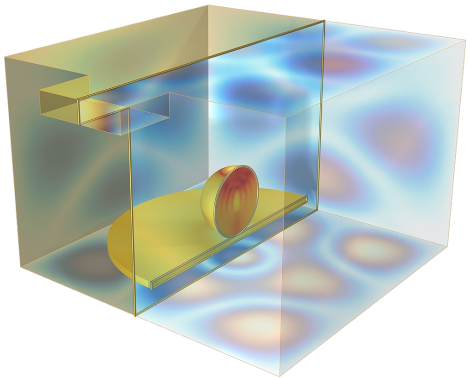
- Involving heterogeneous models
- Requiring significant computational resources
- Problems from data transfer and synchronization
- Error propagation between coupled numerical techniques



EM, thermal, and structural analysis of the microstrip



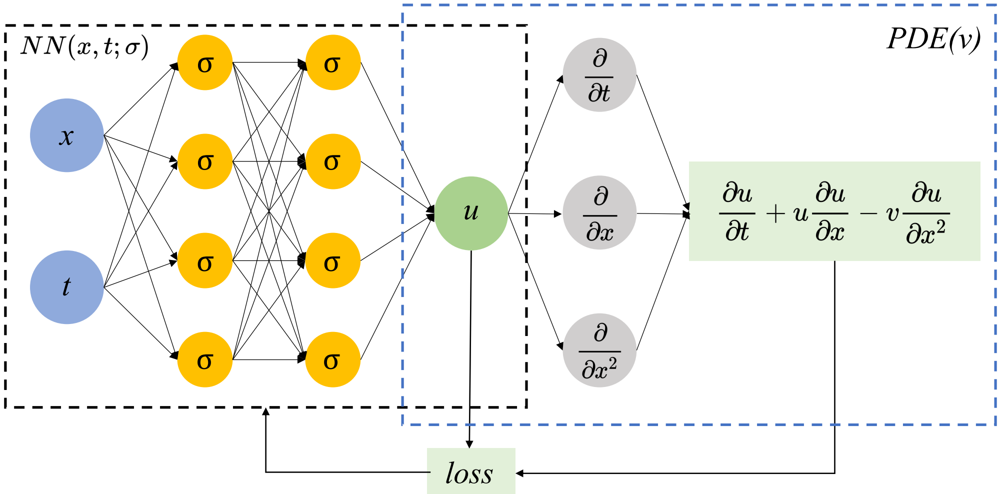
The electric field around an air phantom inside of a birdcage coil



Heat transfer simulations in an microwave oven

# Physics-Informed Neural Networks

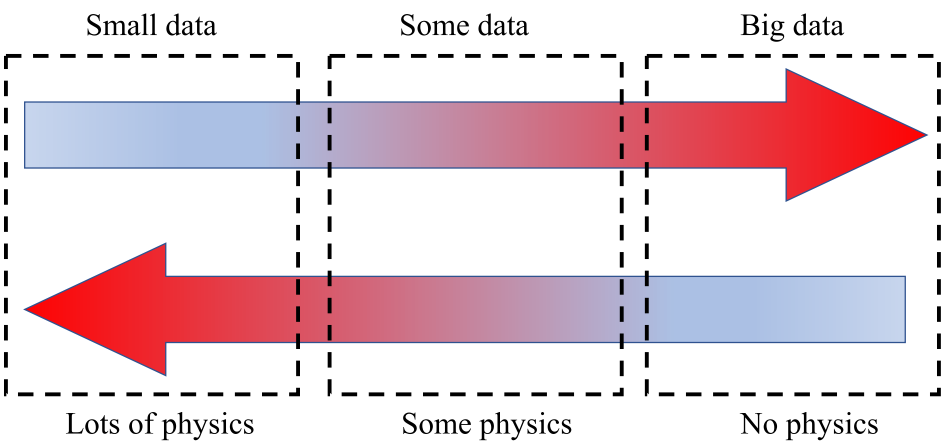





PINN algorithm

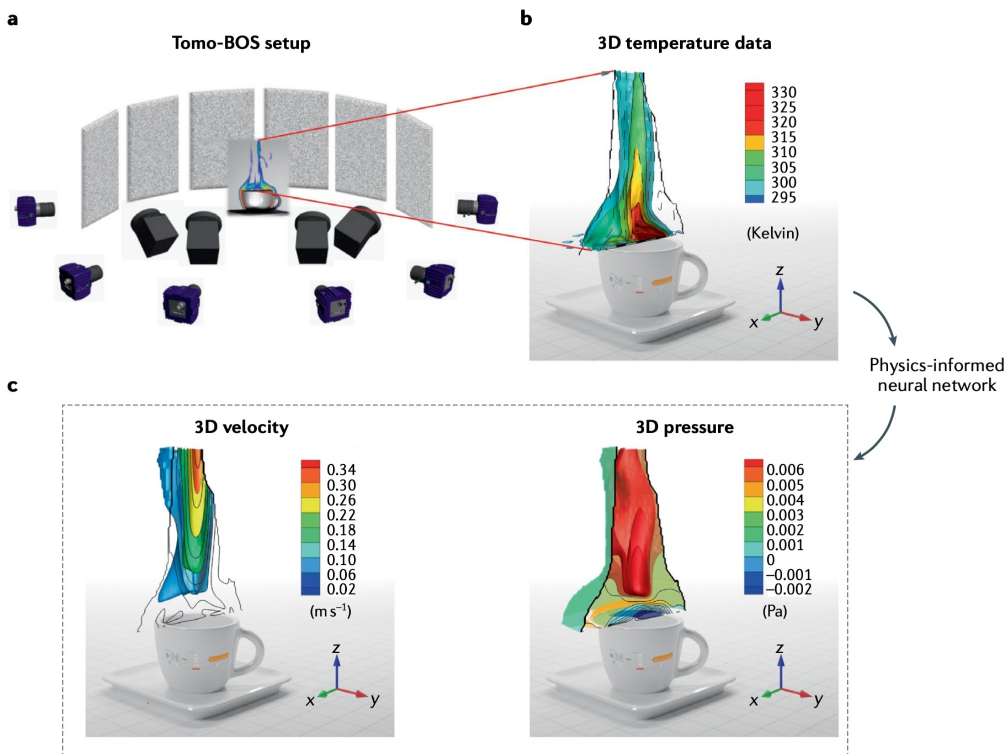
## Key points of state-of-the-art PINN

- Unsupervised training
- Computational efficiency
- Better generalization ability
- Real-world applications

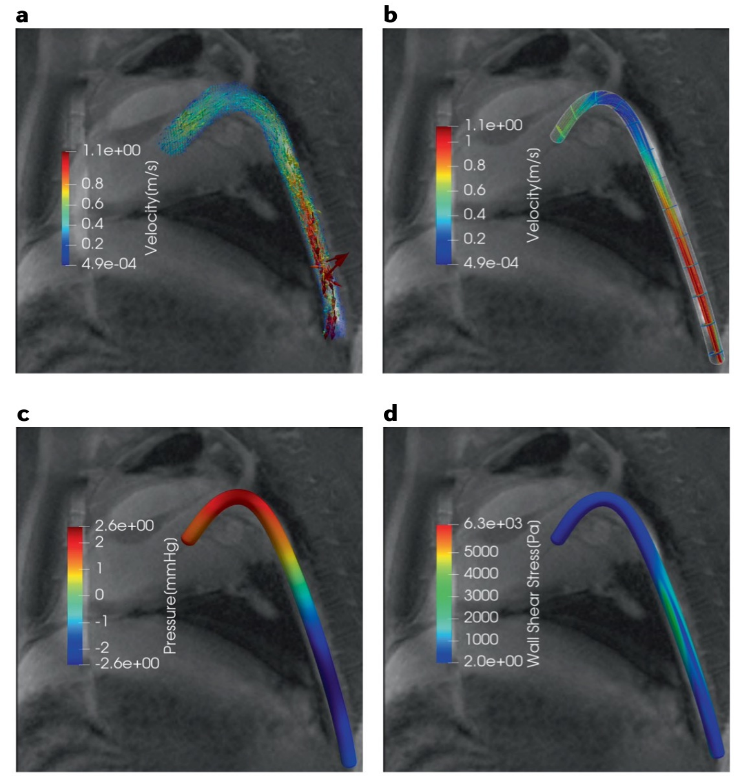



G. E. Karniadakis, I. G. Kevrekidis, L. Lu, P. Perdikaris, S. Wang, and L. Yang, "Physics-informed machine learning," Nature Reviews Physics, vol. 3, no. 6, pp. 422–440, 2021.

# Physics-Informed Neural Networks




Inferring the 3D temperature, velocity, and pressure flow over an espresso cup with PINN.

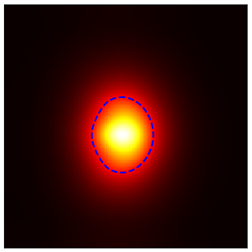



Physics-informed filtering of in-vivo 4D-flow magnetic resonance imaging data of blood flow in a porcine descending aorta.

# Electromagnetic-thermal analysis



Temperature distribution



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FDTD solver for EM and thermal

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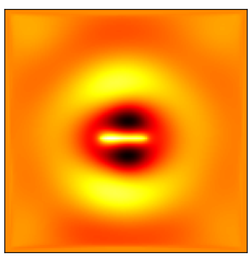


Electric field

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} - \vec{M}$$

$$\frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H} - \vec{J}$$

$$\rho C_p \frac{\partial T}{\partial t} = Q + \nabla \cdot (k \nabla T) + V_s (T_b - T)$$

$$Q = \sigma \left\langle |\mathbf{E}|^2 \right\rangle$$

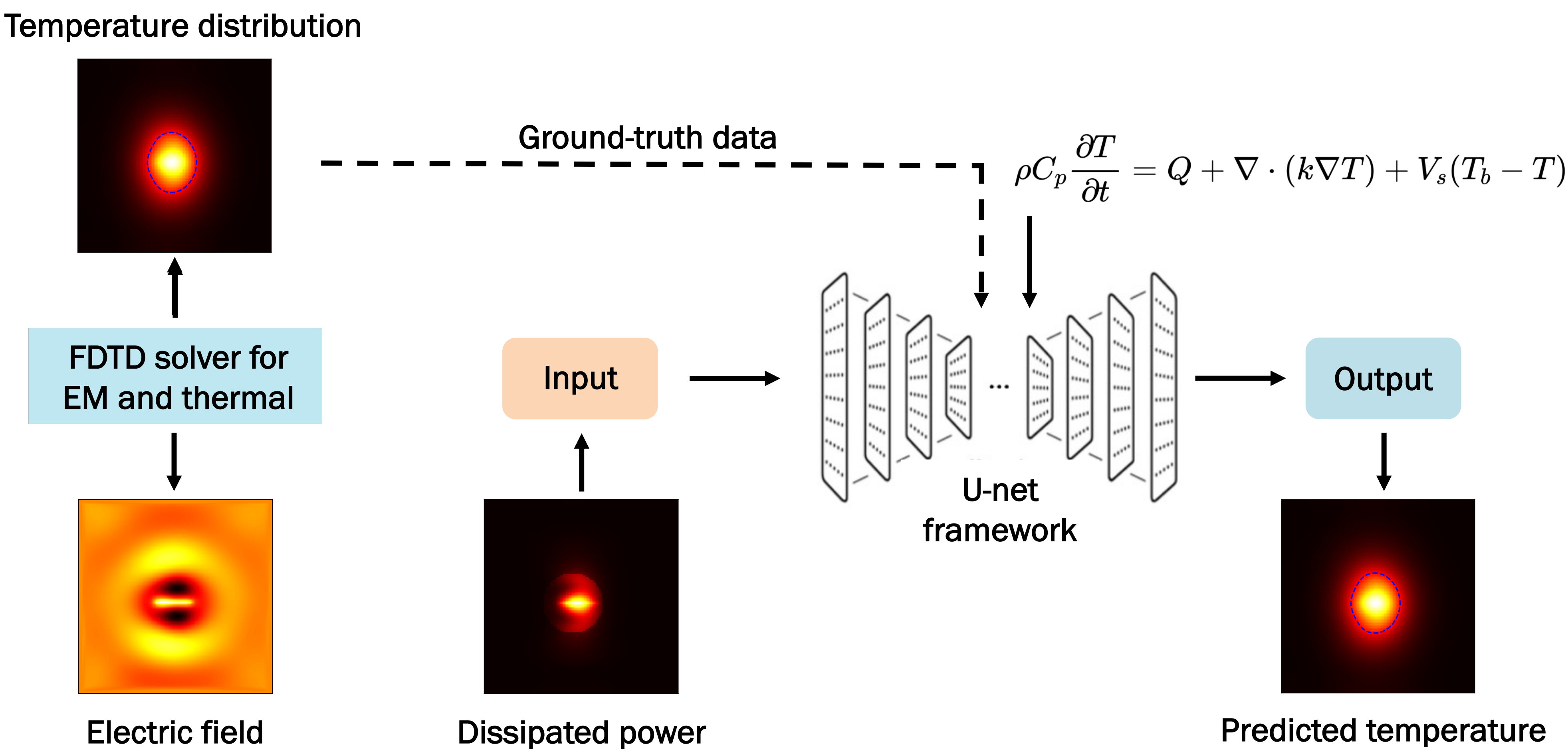
Coupled electromagnetic-thermal problems can be analyzed by numerical solvers, such as FEM and FDTD. However, there are several questions to be addressed:

- Complex mathematical models and enormous computing resources requirement
- Error propagation between coupled multiphysics numerical solvers
- Appropriate spatial discretization for different solvers

Therefore, we combine the robust/well-understood FDTD solver for the electromagnetic simulation with a neural network for the thermal simulation.

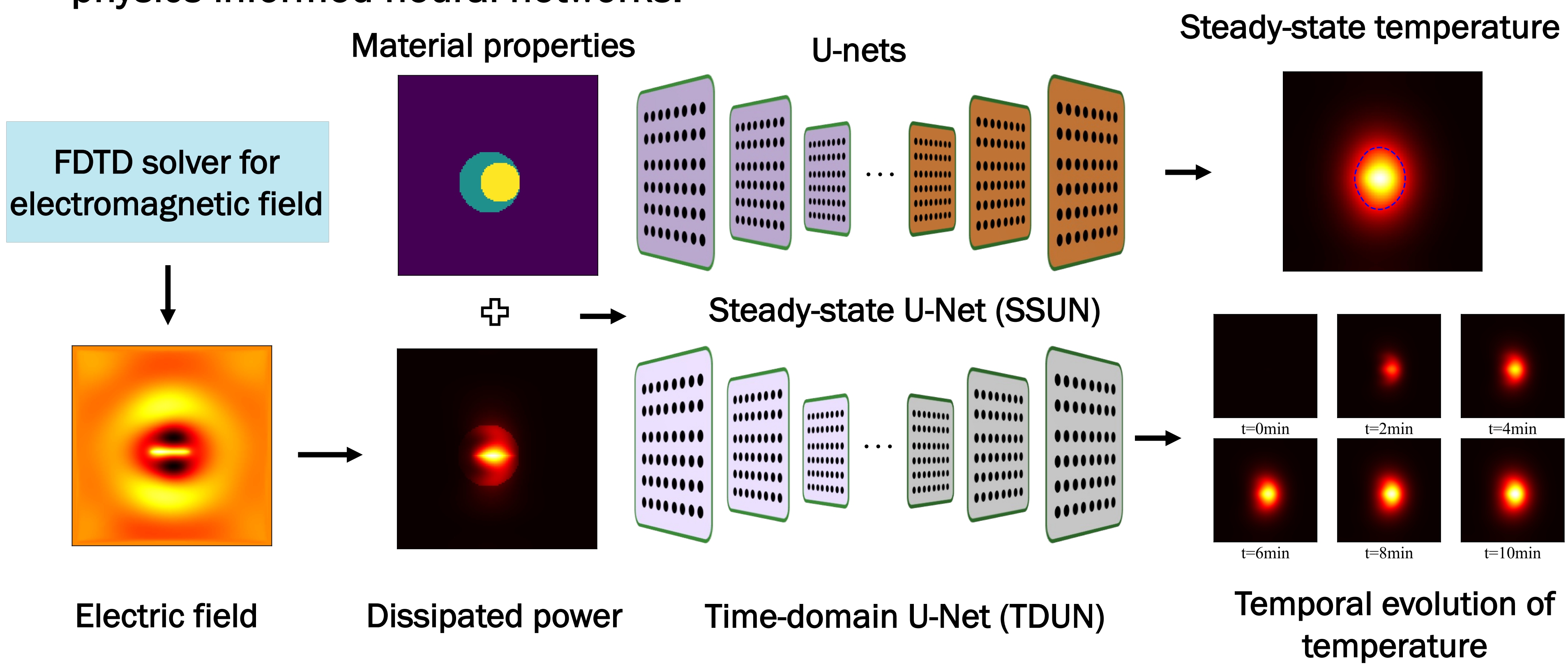
# Electromagnetic-thermal analysis





# PINNs for electromagnetic-thermal simulation

*Goal:* Replace the numerical thermal solver in electromagnetic-thermal simulations with physics-informed neural networks.



# PINNs for electromagnetic-thermal simulation



**Key points:** Implement the heat equation and boundary conditions into the neural networks to enable the unsupervised training.

Heat equation: $$\rho C_p \frac{\partial T}{\partial t} = Q + \nabla \cdot (k \nabla T) + V_s (T_b - T)$$

Approximate the partial derivative of the temperature with respect to time with forward finite difference:

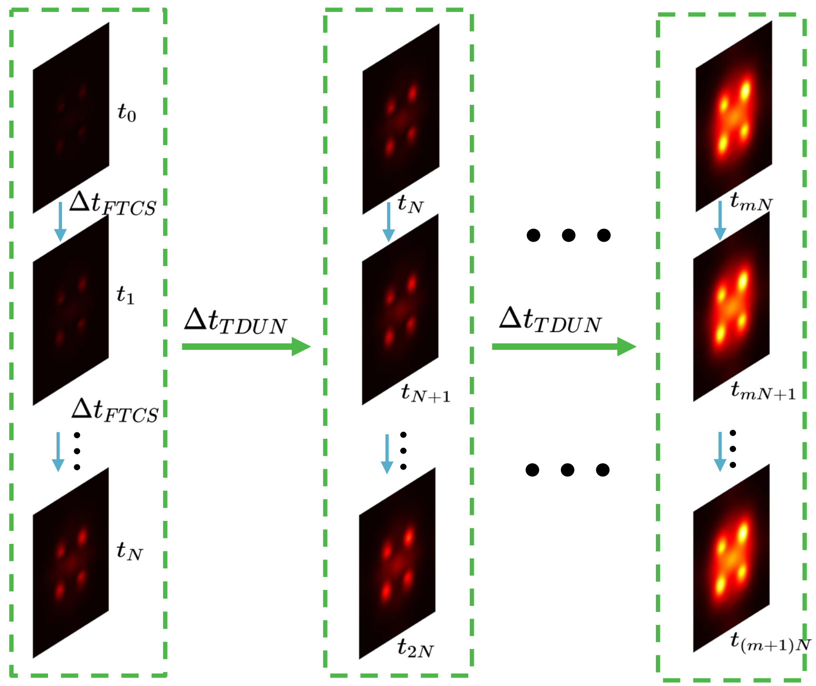
$$T^{n+1} - T^n - \frac{\Delta t_{div}}{\rho C_p} \left( Q + k \nabla^2 T^n + V_s (T_b - T^n) \right) = 0$$

For *N* successive steps:

$$\sum_{i=n}^{n+N-1} \left( T^{i+1} - T^i - \frac{\Delta t_{div}}{\rho C_p} \left( Q + (k \nabla^2 T^i) + V_s (T_b - T^i) \right) \right) = 0$$

Then, the loss function of the TDUN becomes:

$$L_{TDUN} = \sum_{i=n}^{n+N-1} \left| T^i - T^{i+1} + \frac{\Delta t_{div}}{\rho C_p} \left( Q + (k \nabla^2 T^i) + V_s (T_b - T^i) \right) \right|^2$$




Update of FTCS — Update of TDUN

# PINNs for electromagnetic-thermal simulation



*Key points:* Implement the heat equation and boundary conditions into the neural networks to enable the unsupervised training.

Heat equation: $$\rho C_p \frac{\partial T}{\partial t} = Q + \nabla \cdot (k \nabla T) + V_s (T_b - T)$$

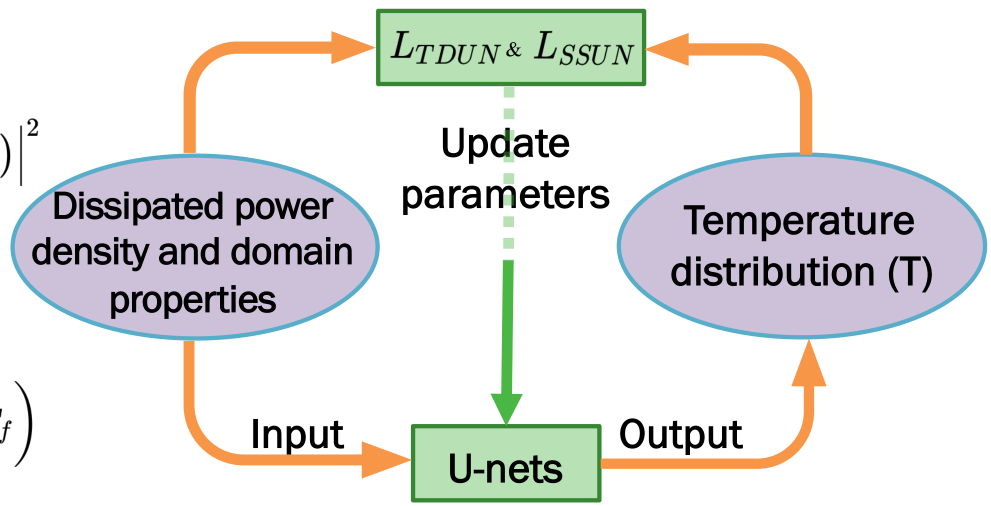
Loss function:

$$L_{TDUN} = \sum_{i=n}^{n+N-1} \left| T^i - T^{i+1} + \frac{\Delta t_{div}}{\rho C_p} \left( Q + (k \nabla^2 T^i) + V_s (T_b - T^i) \right) \right|^2$$

Robin boundary condition: $$-k \left( \frac{\partial T}{\partial \mathbf{n}} \right)_w = h(T_w - T_f)$$

In a discretized form: $$-k \left( \frac{T_{i,j} - T_{i-1,j}}{\Delta x} \right) = h \left( \frac{T_{i,j} + T_{i-1,j}}{2} - T_f \right)$$

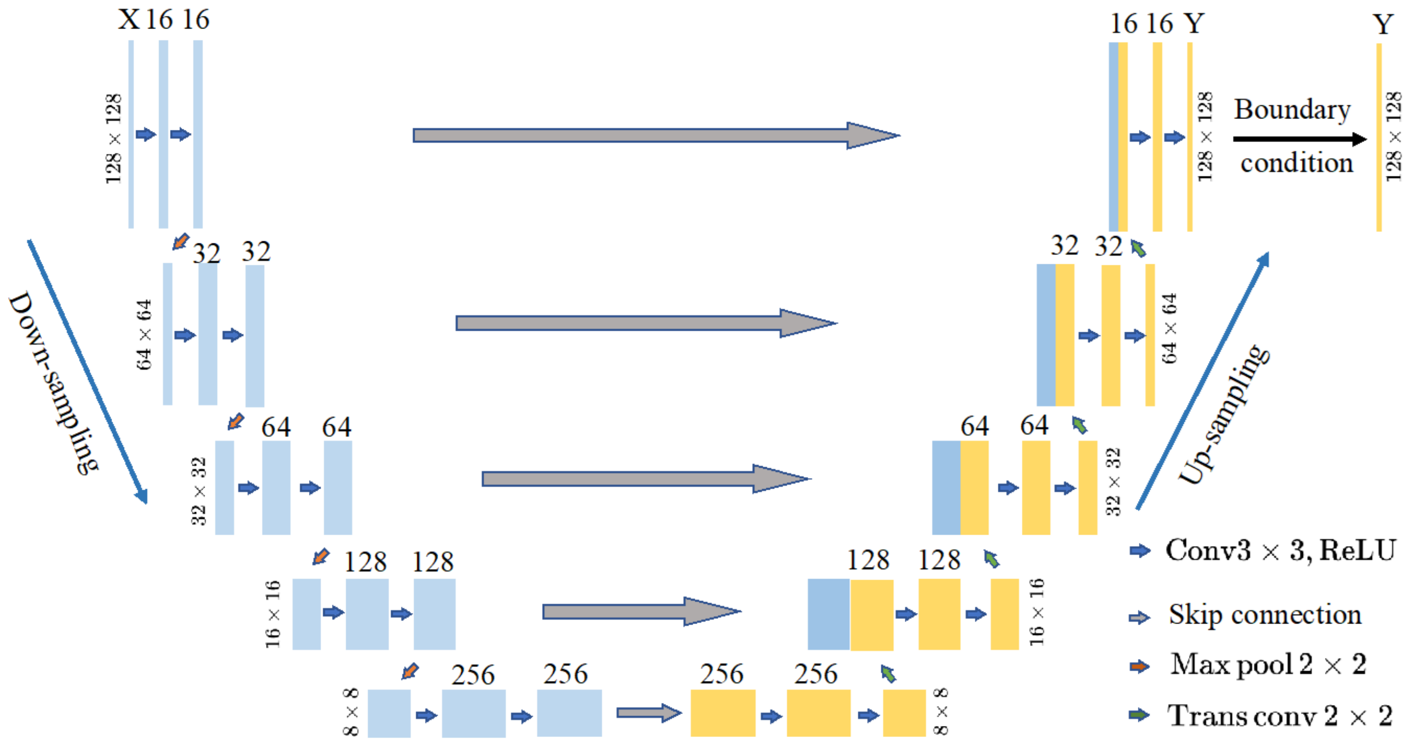
Each element at the boundary: $$T_{i,j} = \frac{(2k - h\Delta x) T_{i-1,j} + 2h\Delta x T_f}{2k + h\Delta x}$$



# PINNs for electromagnetic-thermal simulation

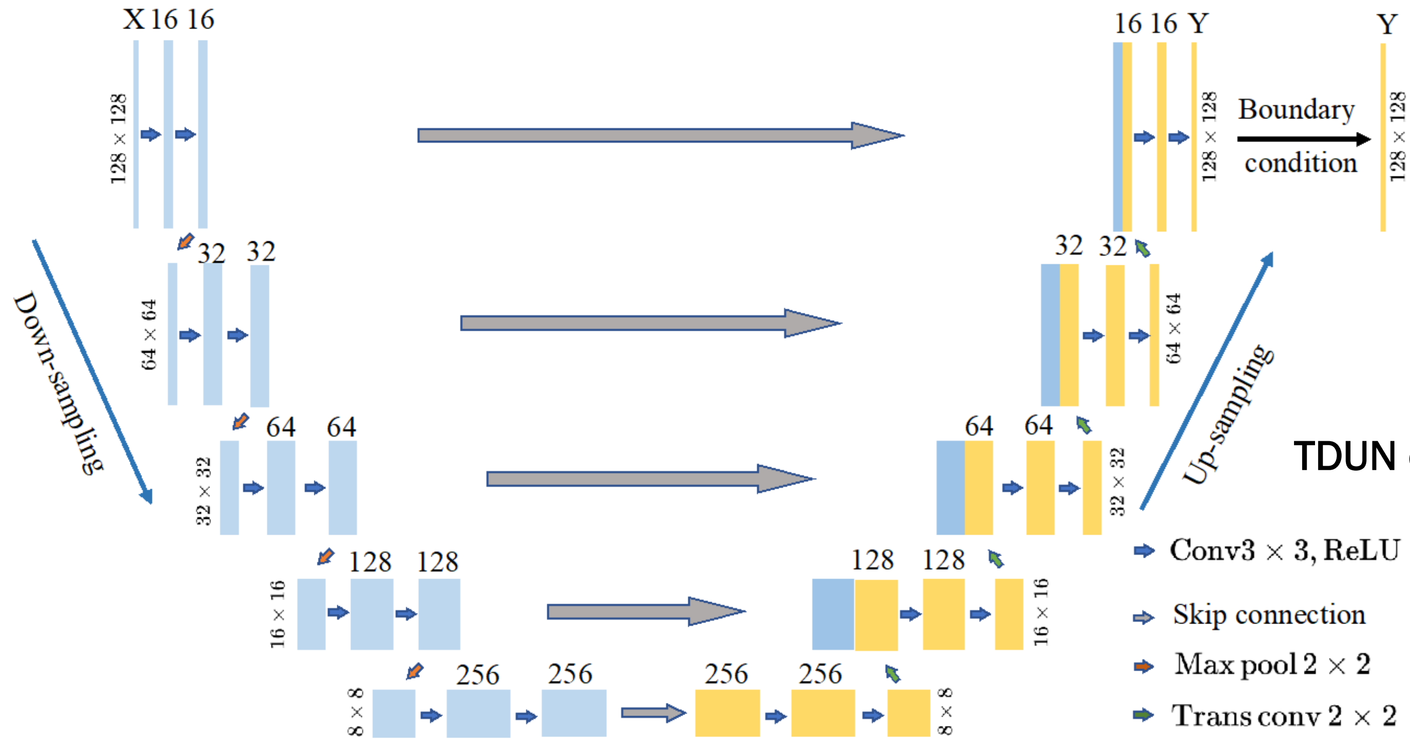


## Details of the U-Net:



# PINNs for electromagnetic-thermal simulation

Details of the U-Net:




TDUN input:

$T^0$: initial temperature distribution (K)

$Q$: dissipated power density (W/$m^3$)

$k$: heat conductivity (W/m/K)

$C_p$: heat capacity (J/kg/K)

$\rho$: material density (kg/$\mathrm{m}^3$)

TDUN output:

$\{T_{i,j}\}^{n=1,2,\ldots,N}$: N successive steps of temperature (K)

# Numerical experiments

Domain settings and materials

Building database

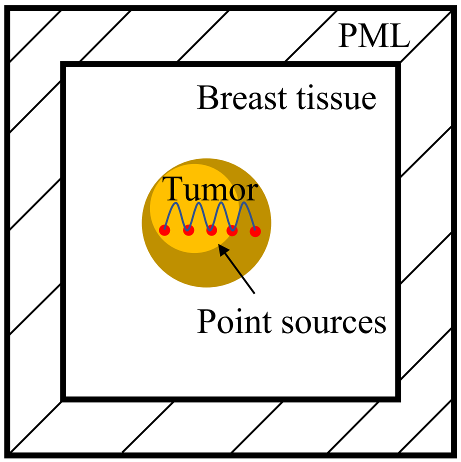
Numerical results

Study of hyperparameters

Discussion of the results

# Numerical experiments - Domain settings and materials






Computational Domain

TABLE I
ELECTRICAL PROPERTIES OF MATERIALS IN THE SIMULATION AT 2 GHz

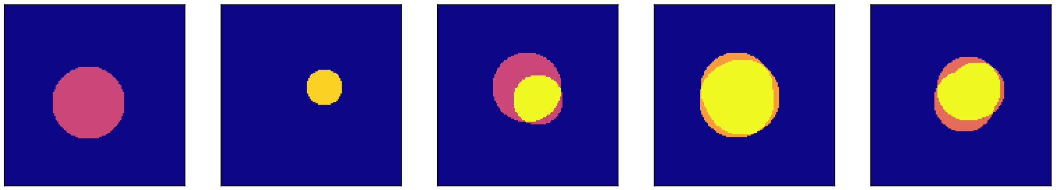
| | Relative Permittivity $\varepsilon_r$ | Relative Permeability $\mu_r$ | Electrical Conductivity $\sigma$(S/m) |
|---|---|---|---|
| Breast tissue | $8.163 \pm 0.577$ | 1 | $0.497 \pm 0.069$ |
| Benign Tumor | $21.664 \pm 1.559$ | 1 | $0.955 \pm 0.122$ |
| Cancer | $63.008 \pm 2.108$ | 1 | $4.164 \pm 0.074$ |

TABLE II
THERMAL PROPERTIES OF MATERIALS IN THE SIMULATION

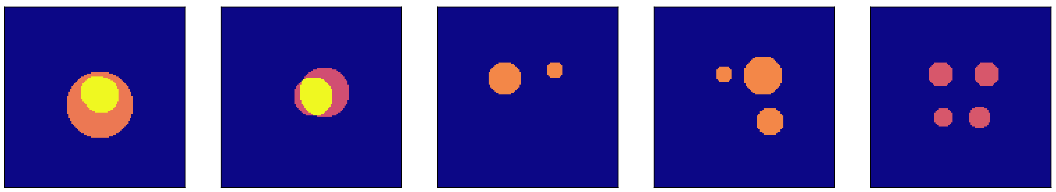
| | Thermal Conductivity $k$(W/m/K) | Heat Capacity $C_p$(J/kg/K) | Density $\rho(\mathrm{kg/m^3})$ |
|---|---|---|---|
| Breast | 0.500 | 3770 | $1000\pm100$ |
| Benign Tumor | $0.580\pm0.02$ | $3600\pm200$ | $1000\pm100$ |
| Cancer | $0.580\pm0.02$ | $3600\pm200$ | $1000\pm100$ |
| Blood | | 3622.5 | $1000\pm100$ |

# Numerical experiments – building database

Training cases



Testing cases



Both training data and testing data include benign and malignant tumors. The induced temperature should be in excess of 323.15 K (50℃) to ablate tumor cells. The source amplitude is set to 300 V/m for benign tumors and 100 V/m for malignant tumors.

Robin boundary condition: $-k\left(\frac{\partial T}{\partial \mathbf{n}}\right)_w = h(T_w - T_f)$

Heat transfer coefficient: $h = 5\mathrm{W/m^2/K}$

$$\rho C_p \frac{\partial T}{\partial t} = Q + \nabla \cdot (k\nabla T) + V_s(T_b - T)$$

Eliminate the temperature of flowing blood:

$$T^{'} = T - T_b$$

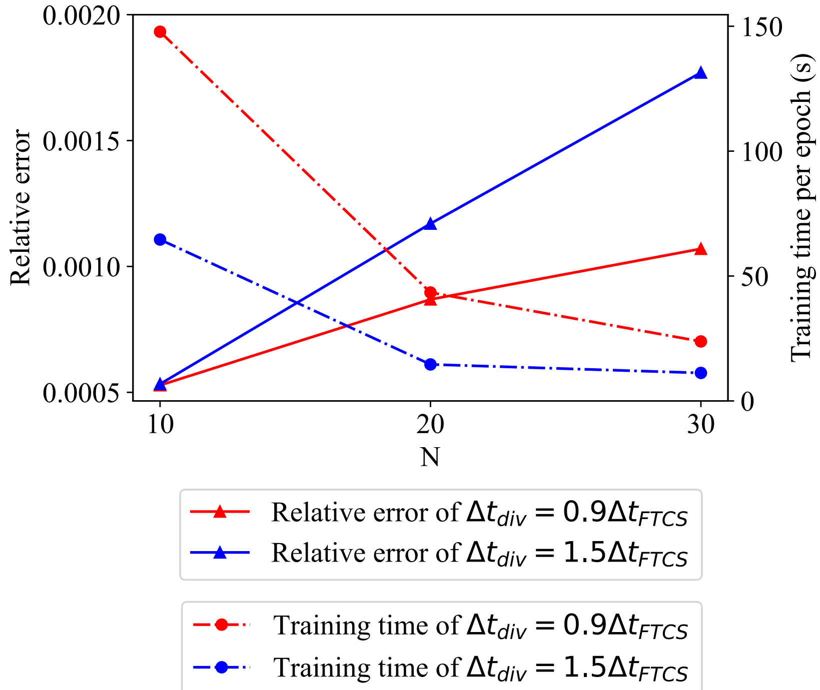
$$\rho C_p \frac{\partial T^{'}}{\partial t} = Q + k\nabla^2 T^{'} - W_b C_b T^{'}$$

Relative error: $\mathcal{E}_{rel} = \frac{1}{128^2}\sum_{i=1}^{128}\sum_{j=1}^{128}\frac{|T_p(i,j) - T_r(i,j)|}{T_r(i,j) - 310}$

# Numerical experiments – study of hyperparameters



## Choice of N and $\Delta t_{div}$

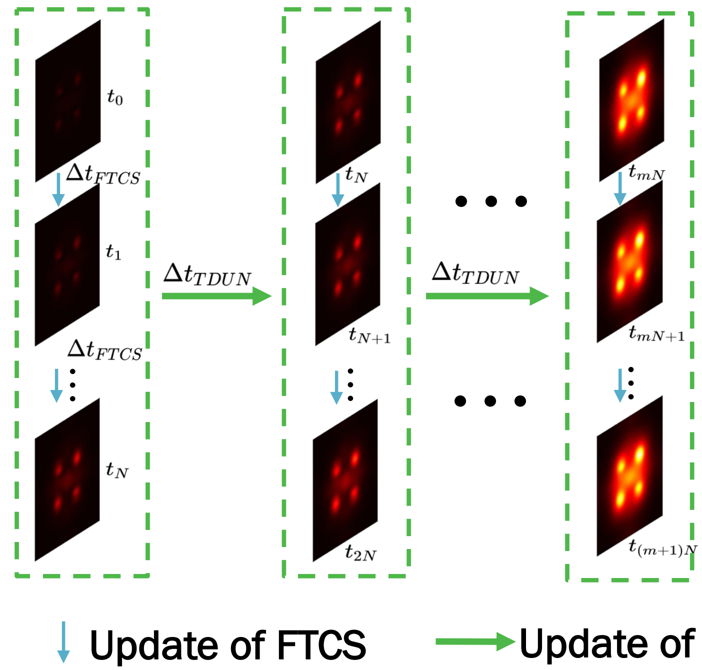



$\Delta t_{FTCS}$: largest time step allowed by the stability limit

N: the number of steps in each batch of TDUN

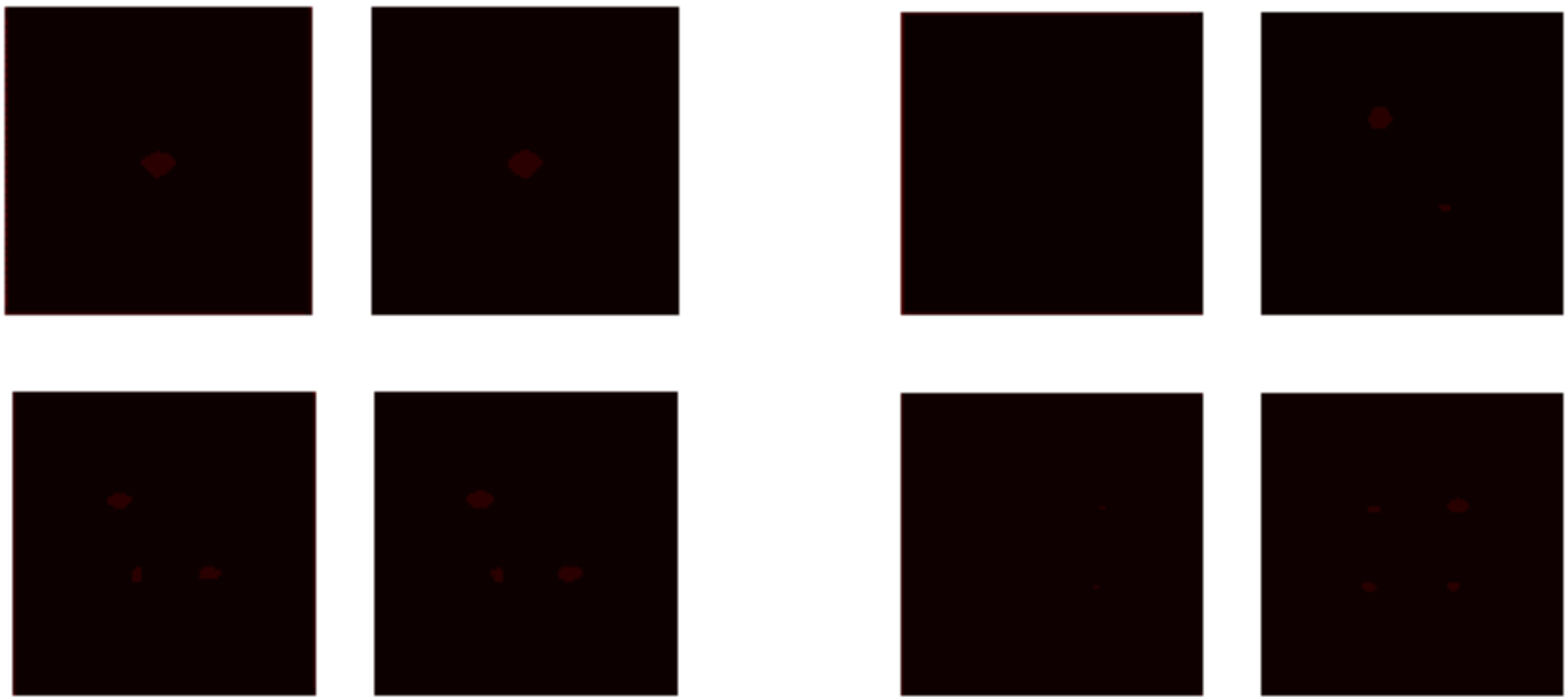
$\Delta t_{div}$: the time step within each batch

$\Delta t_{TDUN} = N \times \Delta t_{div}$: effective time step



# Numerical experiments - Results

TDUN prediction | FTCS ground-truth | TDUN prediction | FTCS ground-truth



# Numerical experiments - Discussion

## Efficiency: compare training time and execution time on an intel-I5 CPU, and Nvidia GTX 3090 GPU

The time step of the TDUN is not limited by the stability condition of finite-difference method, in this work, $\Delta t_{TDUN} = 1.5 \Delta t_{FTCS}$.

TABLE III
COMPARISON OF EXECUTION TIME OF FTCS AND TDUN

| | FTCS (s/case) | TDUN (s/case) |
|---|---|---|
| Intel-i5 CPU | 22.74 | 4.34 |
| NVidia GTX 3090 GPU | / | 1.28 |

## Generalization ability:

Both the SSUN and TDUN is trained based on the embedded heat equation.

They generalize well to:

- Shape of objects
- Number of objects
- Amplitude of the source
- Material properties

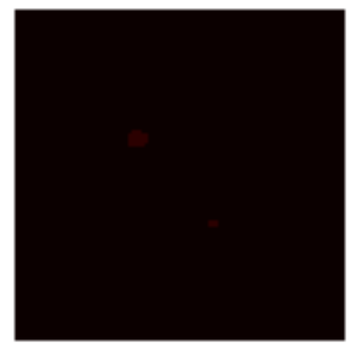
# Conclusion



- Physics-informed U-nets to replace the thermal solvers
- The network is trained in an unsupervised approach, no ground-truth data needed
- Coupled numerical method with neural networks for multiphysics modeling
- Numerical results demonstrate the *accuracy*, *efficiency* and *generalization ability* of the proposed approach

## Future work

- PINN for EM simulation: test & evaluation
- PINN-based 3-D time-domain EM-thermal solver



# Thank you!