Extending the Physics Informed Neural Network Model to Multigroup Neutron Diffusion Problems

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Outline

- Introduction of PINN
- 1G Fixed-source Diffusion Model (M&C 2021)
- 2G Fixed-source Diffusion Model
  - One Dimensional (1D) Examples
  - Two Dimensional (2D) Examples
- Future Work and Conclusions

Physics-Informed Neural Networks (PINN)

- Provides a framework for integrating physics principles within data-driven models
- Solves two classes of problems:
    1. Data-driven solution of PDEs (Forward approach)
    2. Data-driven discovery of PDEs (Inverse approach)
- Successfully applied to various engineering problems:

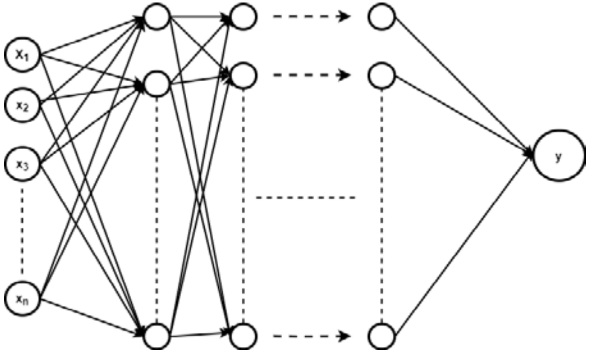
    Fluids, Quantum Mechanics, Power Systems, etc.

Ref.: M. Raissi et al., "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations," *Journal of Computational Physics*, **378**, pp. 686-707 (2019).

Standard Feed-forward Neural Networks

- Universal function approximators

- Automatic differentiation (AD)



Forward PINN Framework

The PINN approach uses the neural networks (NN) model to approximate the solution of PDEs:

- Considering a general non-linear differential operator:

$$F := \mathbb{N}\left(Y(x_1, x_2, \cdots, x_n)\right) = 0$$

- The solution can be approximated to a NN model:

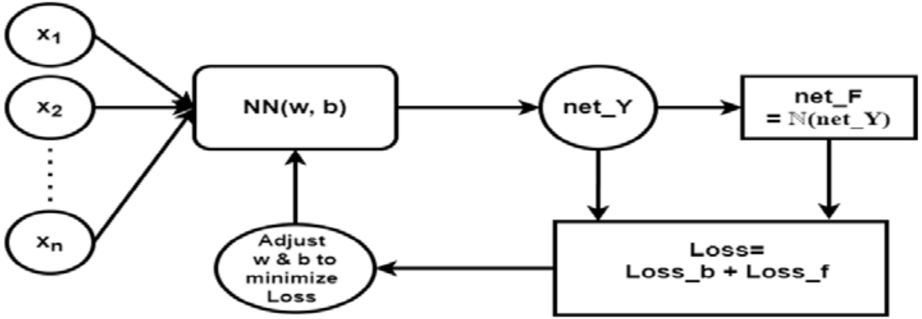
$$Y(x_1, x_2, \cdots, x_n) \cong net\_Y(x_1, x_2, \cdots, x_n)$$

- The PDE model can be constructed as:

$$net\_F := \mathbb{N}\left(net\_Y(x_1, x_2, \cdots, x_n)\right) \cong 0$$

- The shared learnable parameters can be learned by restricting the predictions of (***net_F***) to zero

Forward PINN Framework (Cont.)



PINN Training Scheme

$$\mathbf{Loss} = \underbrace{\frac{1}{N_b}\sum_{i=1}^{N_b}\left[net\_Y(x_1^i, x_2^i, \ldots x_n^i) - Y(x_1^i, x_2^i, \ldots x_n^i)\right]^2}_{\text{Boundary Conditions}} + \underbrace{\frac{1}{N_f}\sum_{i=1}^{N_f}\left[net\_F(x_1^i, x_2^i, \ldots x_n^i)\right]^2}_{\text{Neutron Balance (i.e., physics principle)}}$$

Boundary Conditions

Neutron Balance
(i.e., physics principle)

1G Fixed-source Diffusion Model

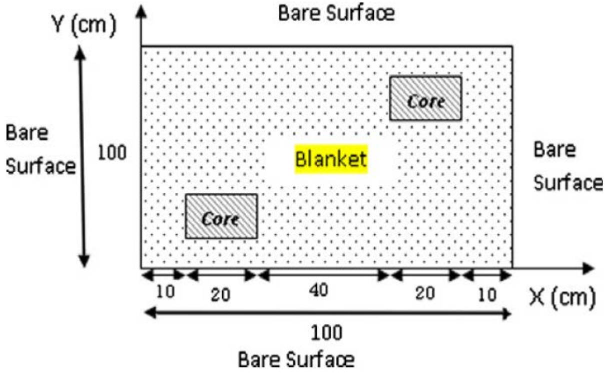
- **The 1G 2D steady state diffusion equation:**

$$\boldsymbol{F} \coloneqq -\nabla \cdot \left(D(x,y)\nabla\phi(x,y)\right) + \Sigma_a(x,y)\phi(x,y) - S(x,y) = 0$$

- **Zero-incoming fluxes are assumed for all boundary surfaces:**

For exmaple, at the surface $x = 0$:

$$\frac{1}{4}\phi(0,y) - \frac{1}{2}D\left.\frac{d\phi}{dx}\right|_{x=0} = 0$$



Geometry of one-group example

Region Material	Σ_a (cm^{-1})	Σ_s (cm^{-1})	S (n/cm^3)
Core	0.062158	0.089302	0.01048083
Blanket	0.064256	0.094853	0.00214231

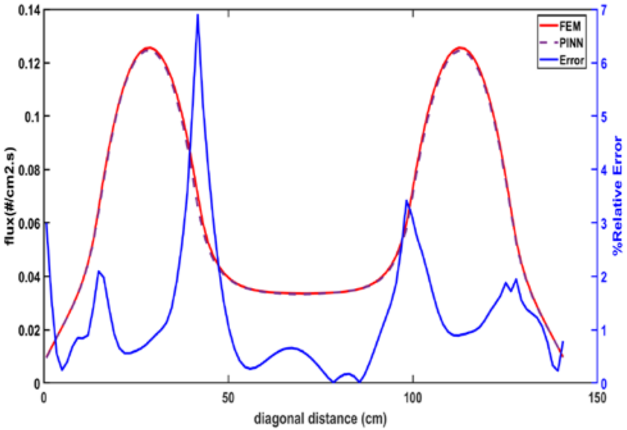
1G Model - Implementation Details

- LHS strategy was used to generate training points
- Adam optimizer was used to minimize the loss function
- A high-order FEM solution was used as a reference solution
- PINN optimum hyperparameters (after optimization)

# of hidden layers	# of neurons/layer	N_f	N_b/surface
8	40	10,000	100

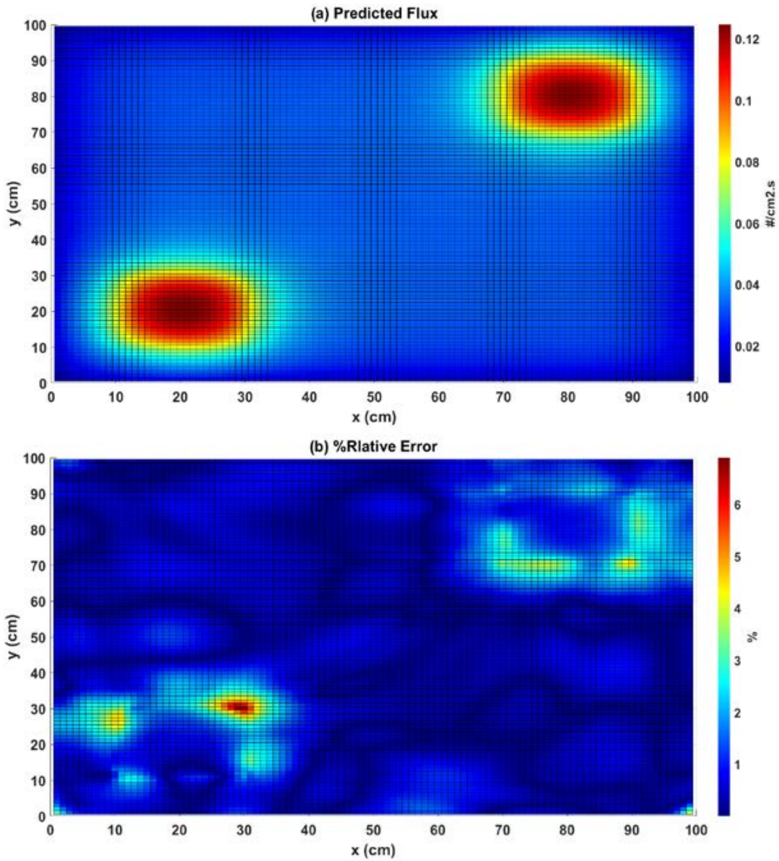
The optimum hyperparameters are shown below with mean percentage relative error of 0.69% and maximum error of 6.9% in flux solution.

1G Model - Results



Predicted flux and percentage relative error along the diagonal line.

Relative percentage error	
Mean	0.69%
Std.	0.74
Max	6.9%



PINN predicted flux distribution (a) and relative percentage error distribution compared to the FEM solution (b).

2G Fixed-source Diffusion Model

$$\begin{cases} f_1 := -\nabla(D_1 \nabla\phi_1) + \Sigma_{r,1}\phi_1 - \nu\Sigma_{f,2}\phi_2 - Q_1 = 0 \\ f_2 := -\nabla(D_2 \nabla\phi_2) + \Sigma_{a,2}\phi_2 - \Sigma_{s,1\to 2}\phi_1 \quad = 0 \end{cases}$$

- **Why it's different?**
  - **Joint learning task**
  - **Generally multi-scale optimization problem**

$$\begin{bmatrix} \phi_1(x,y) \\ \phi_2(x,y) \end{bmatrix} = NN(x,y)$$

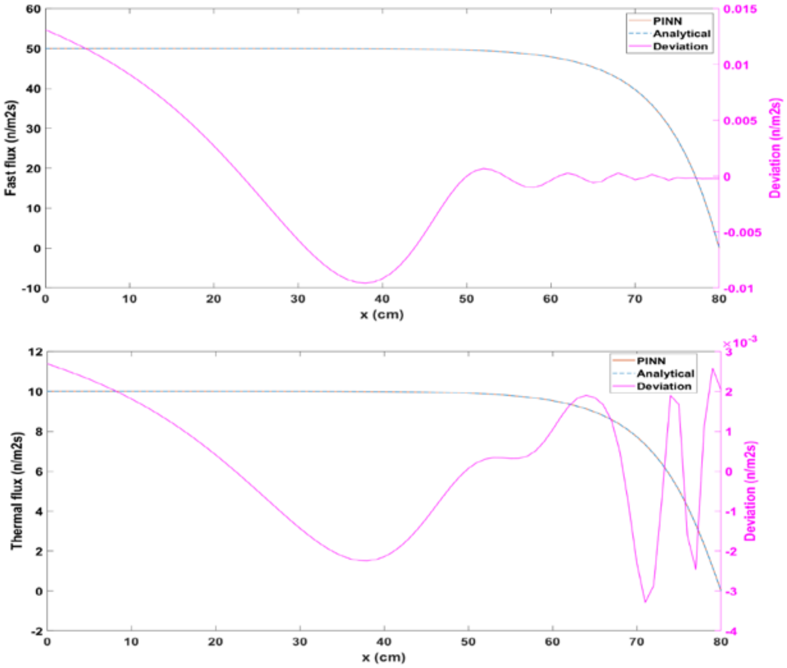
$$\text{Loss} = \underbrace{\sum_{j=1}^{N_b} \left| \begin{matrix} f_{T1}(x_j^T, y_j^T) \\ f_{T2}(x_j^T y_j^T, \end{matrix} \right|^2}_{\text{Boundary Conditions}} + \underbrace{\sum_{i=1}^{N_f} \left| \begin{matrix} f_1(x_i^f, y_i^f) \\ f_2(x_i^f, y_i^f) \end{matrix} \right|^2}_{\text{Neutron Balance}} + \cdots$$

2G1D Exemple - Homogenous Slab

- A **80-cm** thick slab is composed of a single material.
- BCs:
  - Reflective BC on left
  - Zero-flux BC on right

D_1 (cm)	D_2 (cm)	$\Sigma_{r,1}$ (cm^{-1})	$\Sigma_{a,2}$ (cm^{-1})	$\Sigma_{s,1\to2}$ (cm^{-1})	Q_1 $(\mathrm{cm}^{-3}\mathrm{s}^{-1})$
1.2	0.4	0.03	0.1	0.02	1.5

- MAE results:
  - Fast flux: **4.3E-3**
  - Thermal flux: **1.4E-3**



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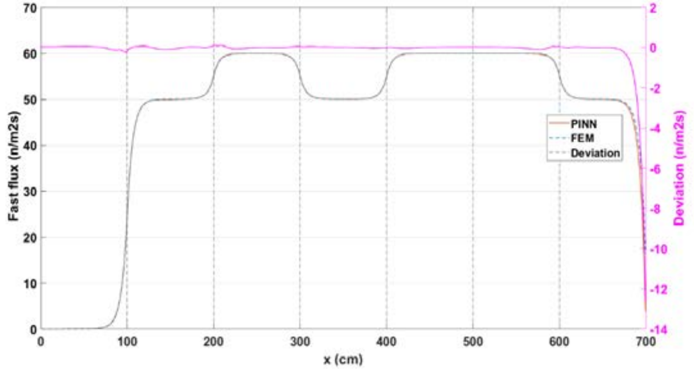
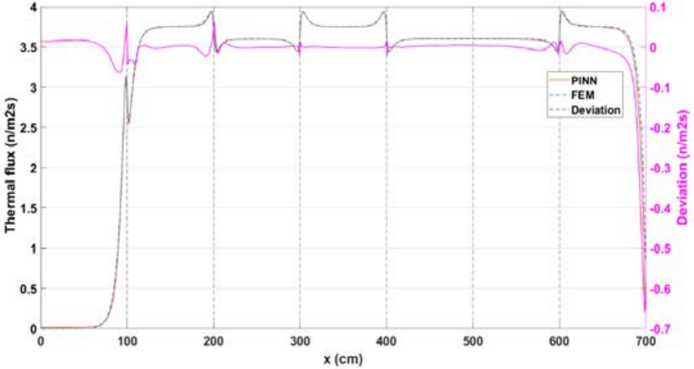
2G1D Exemple – Heterogeneous Slab

- Seven **100-cm** thick assemblies
- Material arrangement: **1-2-3-2-3-3-2**
- BCs:
  - Zero-flux BC for both sides

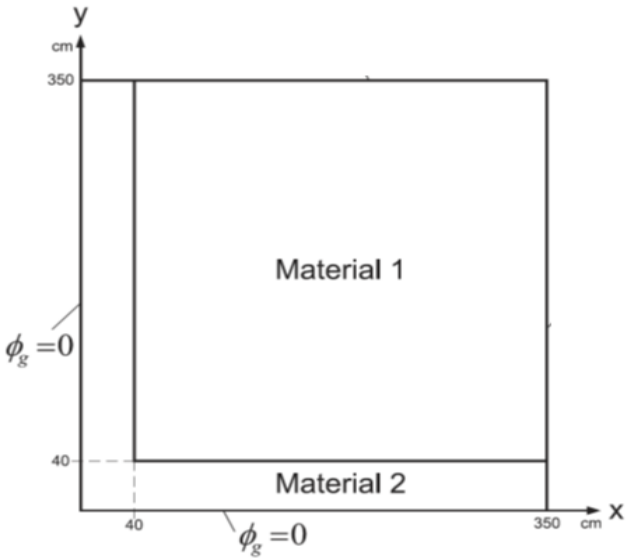
Materials	D_1 (cm)	D_2 (cm)	$\Sigma_{r,1}$ (cm^{-1})	$\Sigma_{a,2}$ (cm^{-1})	$\Sigma_{s,1\to 2}$ (cm^{-1})	Q_1 $(\mathrm{cm}^{-3}\mathrm{s}^{-1})$
1	1.2	0.4	0.03	0.1	0.02	0
2	1.2	0.4	0.03	0.2	0.015	1.5
3	1.2	0.4	0.03	0.25	0.015	1.8

- MAE results:
  - Fast flux: **1.54E-1**
  - Thermal flux: **1.52E-2**





2G2D Exemple – Problem Description

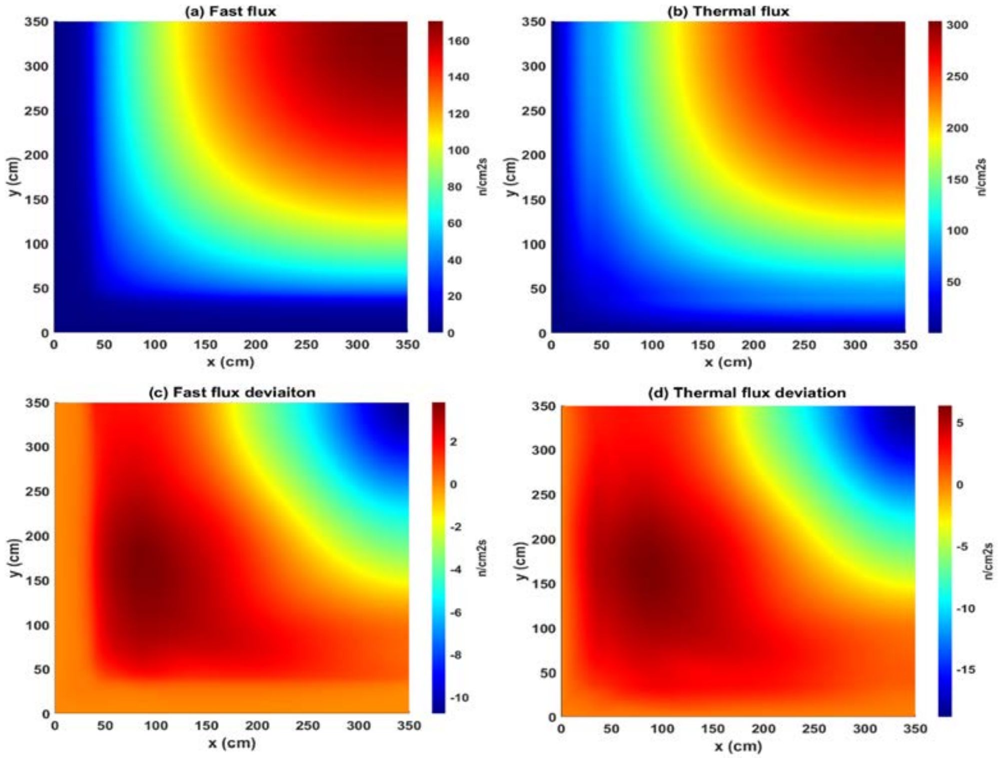


	Material 1	Material 2
D_1 [cm]	1.269	1.31
D_2 [cm]	0.9328	0.8695
$\Sigma_{a,1}$ $[cm^{-1}]$	7.86E-4	0
$\Sigma_{a,2}$ $[cm^{-1}]$	4.1E-3	2.117E-4
$\Sigma_{s,1\to2}$ $[cm^{-1}]$	7.368E-3	1.018E-2
$\nu\Sigma_{f,2}$ $[cm^{-1}]$	4.562E-3	0
Q_1 $[cm^{-3}s^{-1}]$	0.01	0

BCs:

- Reflective BC on right & top
- Zero-flux BC on left & bottom

2G2D Exemple – Flux Distribution

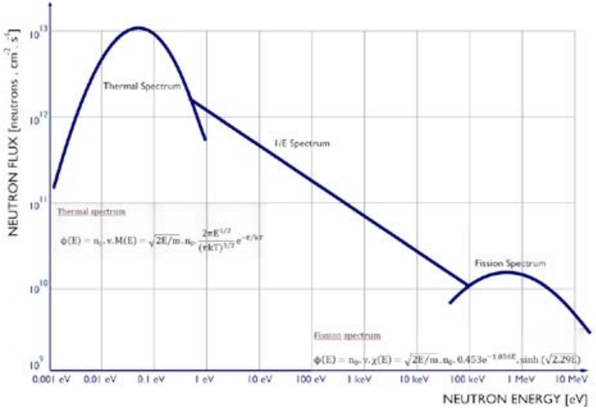


- MAE results:
  - Fast flux: **2.13**
  - Thermal flux: **3.98**

- Considering the average flux value for the fast and thermal groups, the relative error values are within the **3%** and **2%** range, respectively

Future Work

- **Multigroup (G>2) Challenges**
  - *Operator stiffness*
  - *Computational cost*



- ***k*-eigenvalue Problem Challenges**

$$F := \frac{1}{k}\nu\Sigma_f(x,y)\phi(x,y) + \left[\frac{\partial}{\partial x}\left(D\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial\phi}{\partial y}\right)\right] - \Sigma_a(x,y)\phi(x,y) = 0$$

  - *Parametric equation (unknown **k**)*
  - *Homogenous (Direct minimization of **F** results in $\phi(x,y) = 0$)*

Conclusions

- **Advantages:**
  1. Obtain **mesh-free** solutions
  2. **No large amount of training data needed ahead**
  3. Achieve the same level of accuracy as conventional methods.
  4. Manpower efforts for the PINN can be significantly reduced.
- **Challenges:**
  1. Computational complexity
  2. Applications to higher dimensionality problems
  3. Multi-scale optimization

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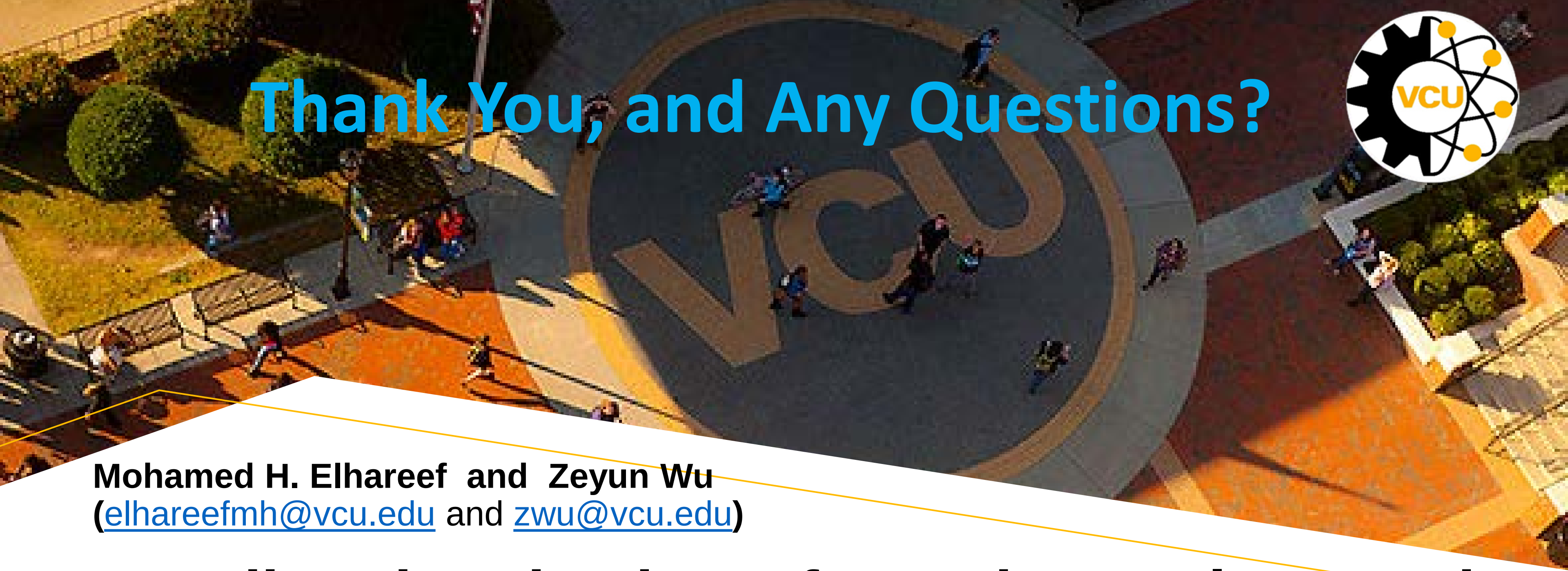
Thank You, and Any Questions?



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