



# SciTech 2025 Vision 2040

1/09/2025



## **Accelerating Large Multiscale Composite Simulations with a GNN/LSTM Microscale Surrogate**

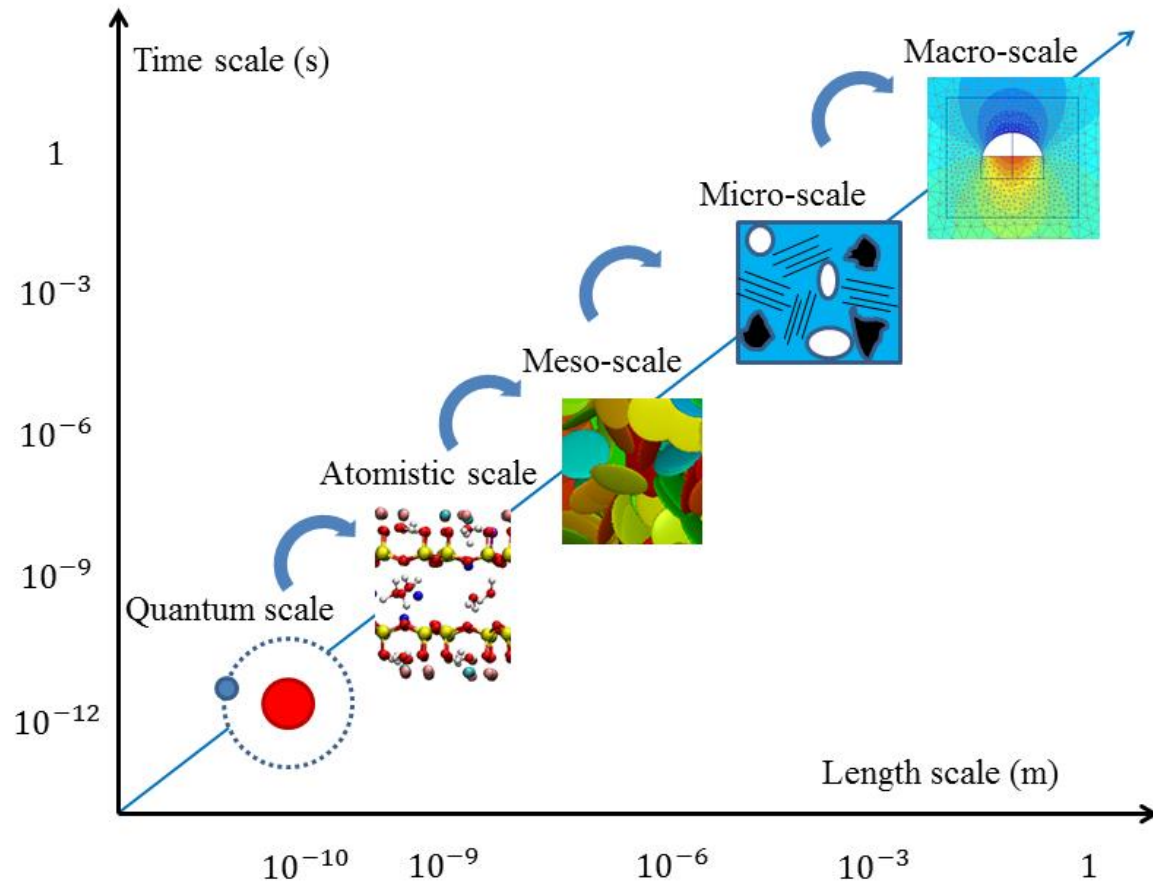
Joshua Stuckner,  
Trenton M. Ricks, Brandon Hearley, Steven M. Arnold

NASA Glenn Research Center



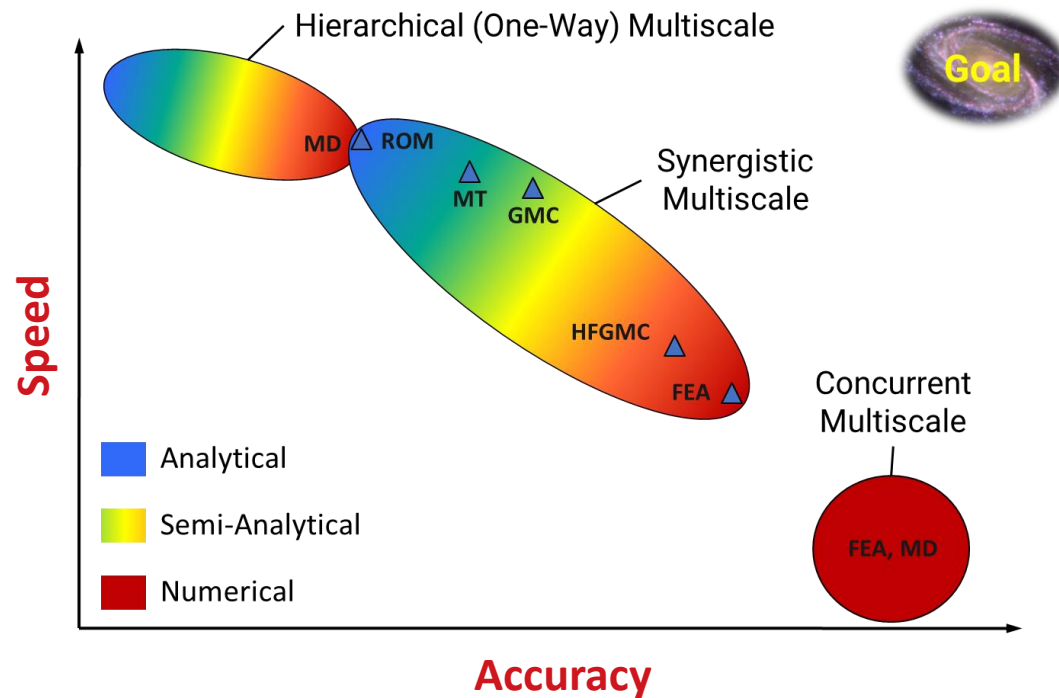
Modeling reduces the need  
for **expensive** physical  
experiments

# Motivation



Multiscale modeling is often required to capture relevant physical effects that span broad time and spatial scales

# Motivation



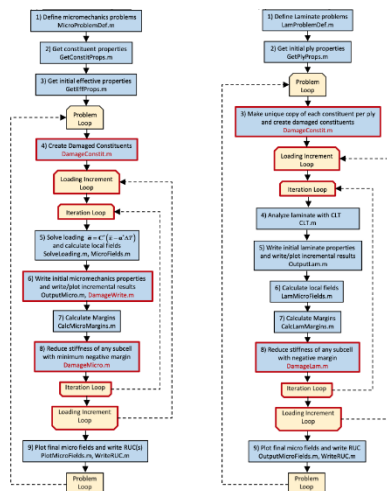
Multiscale models must strike a balance between **speed and accuracy**

# Motivation



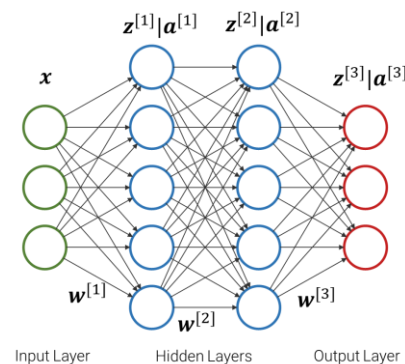
Modeling reduces the need for **expensive** physical experiments

## Physics Model



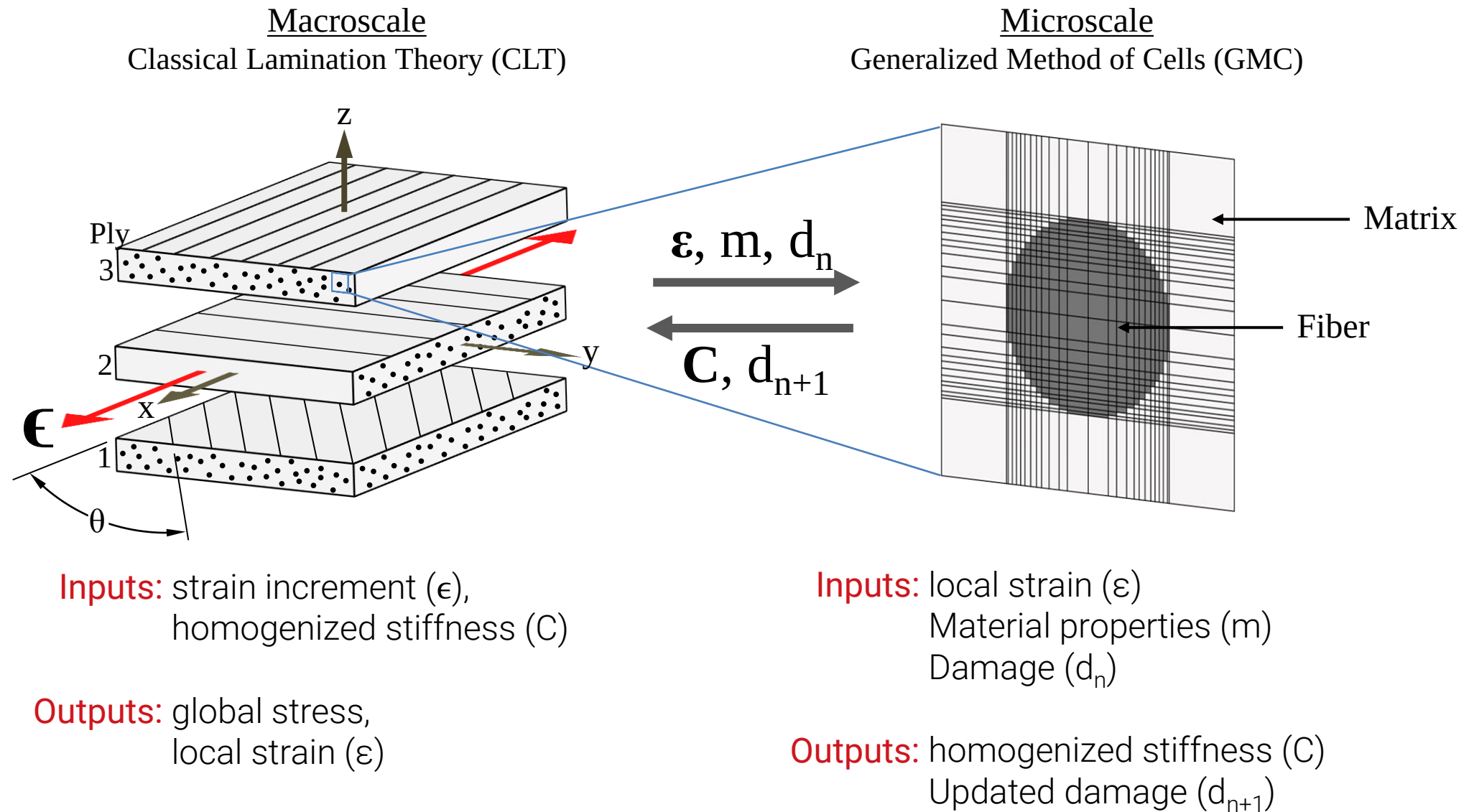
## Neural Network

$$a_i^{[l]} = \max \left( \sum_{j=1}^n (a_j^{[l-1]} w_{ij}^{[l]}) + b_i^{[l]}, 0 \right)$$

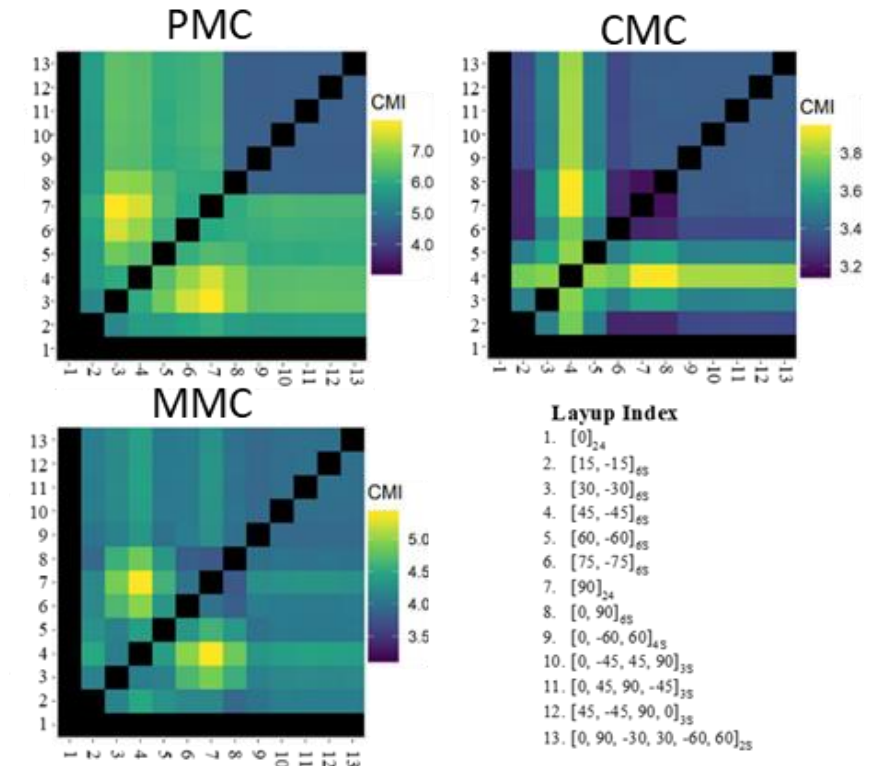
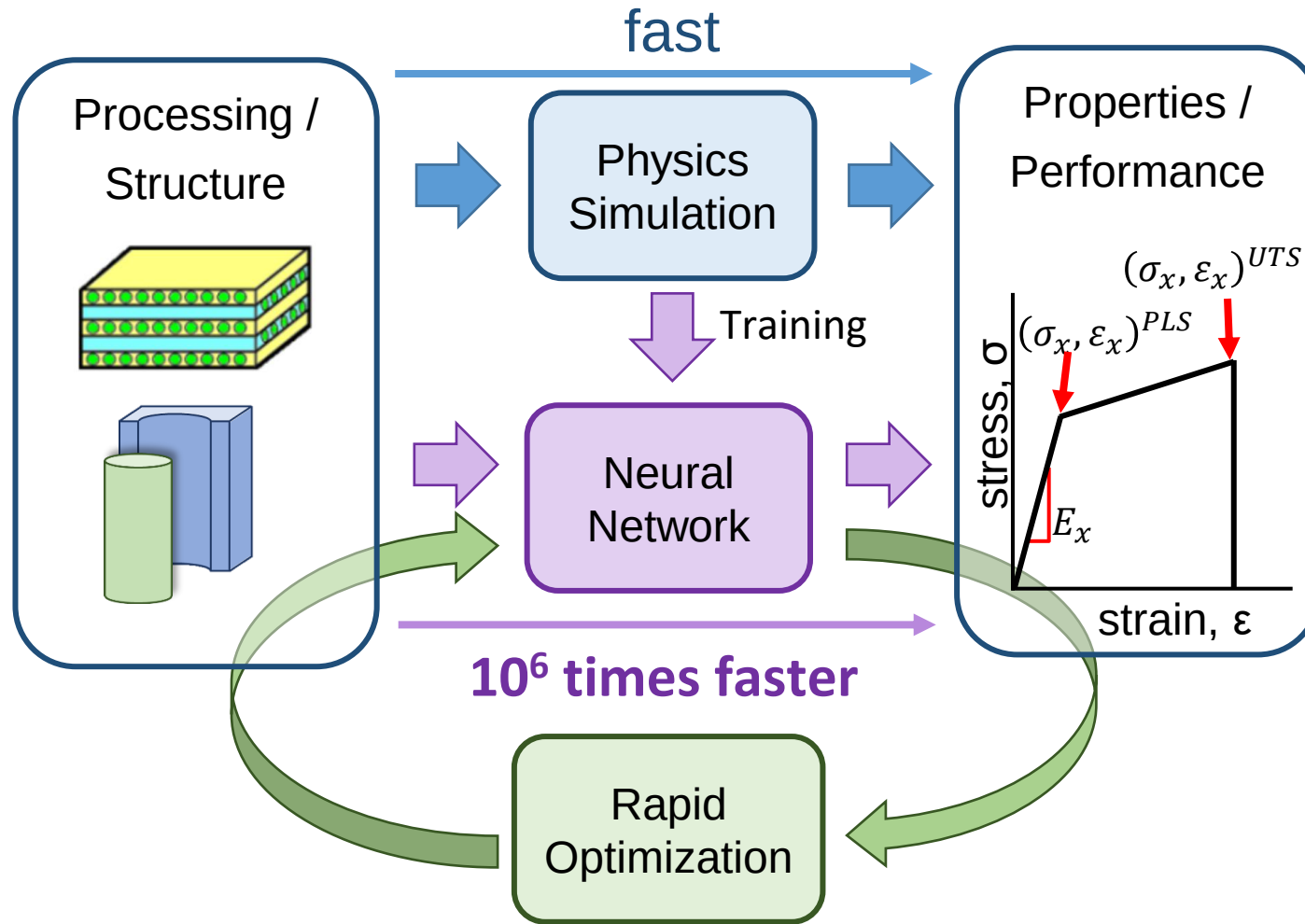


Machine Learning reduces the need for **expensive** modeling

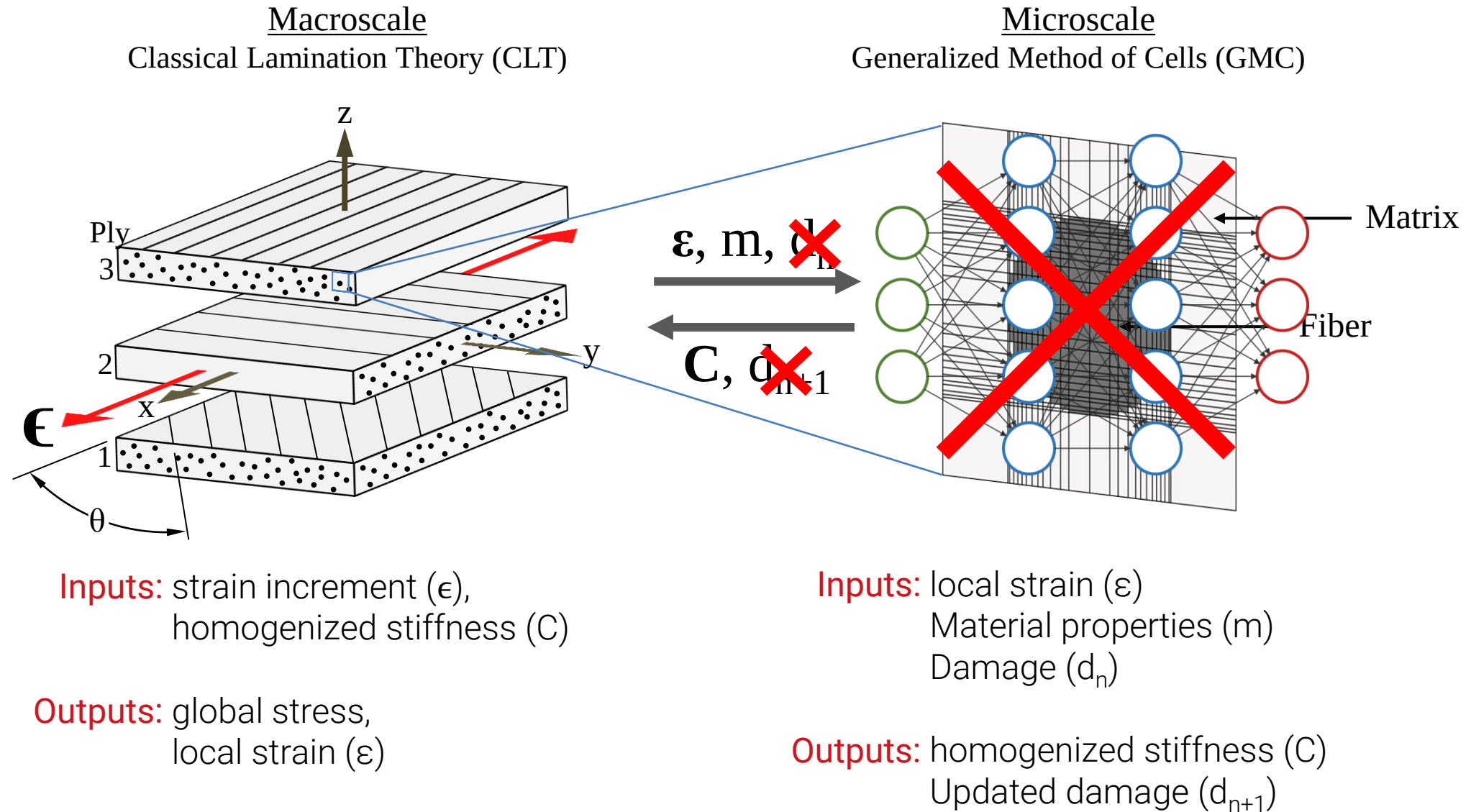
# Composite Model



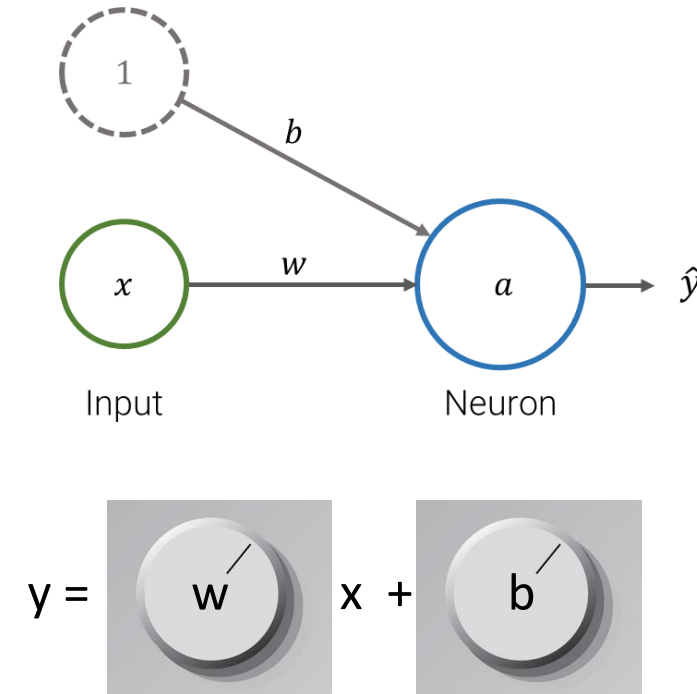
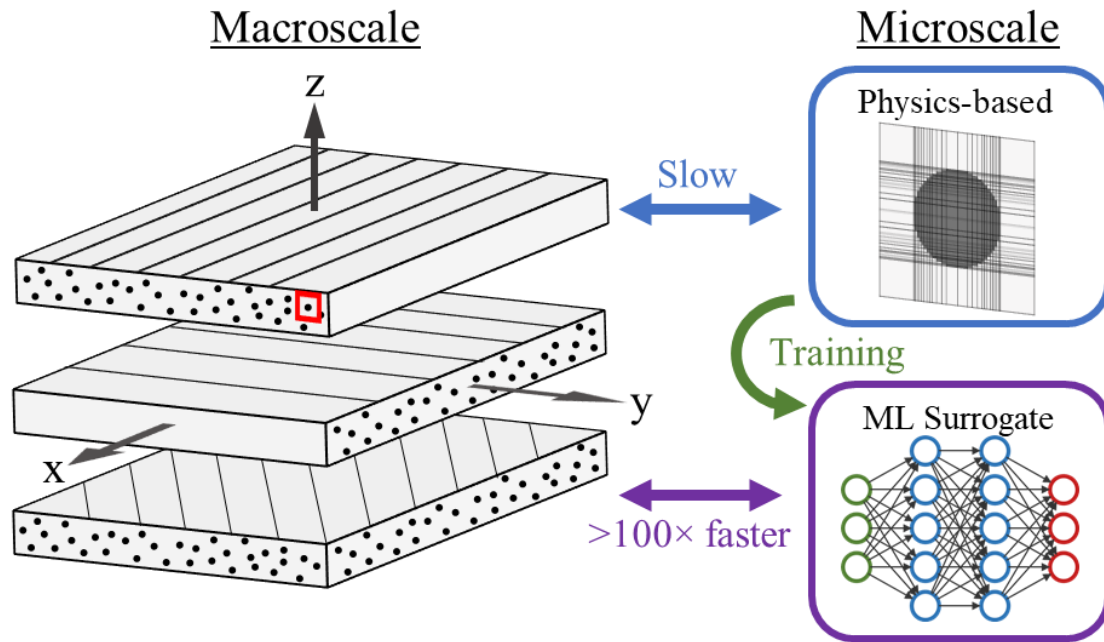
# ML Model



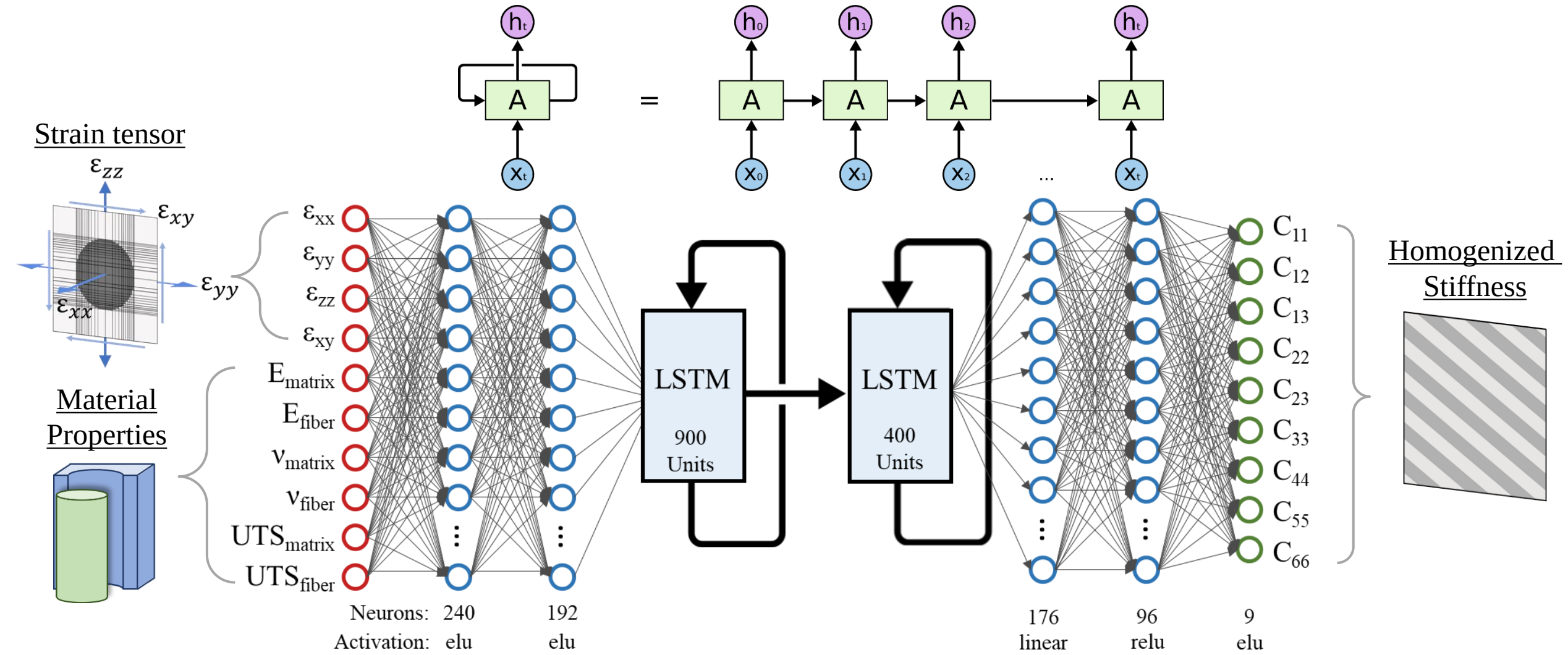
# Microscale Surrogate



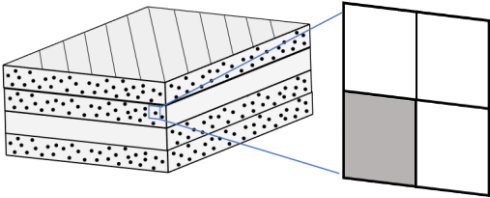
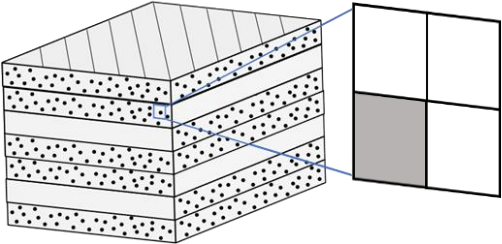
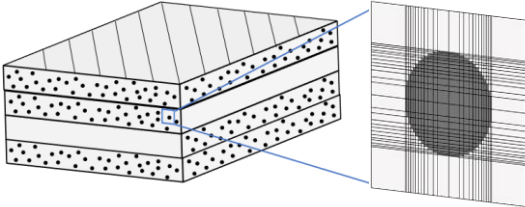
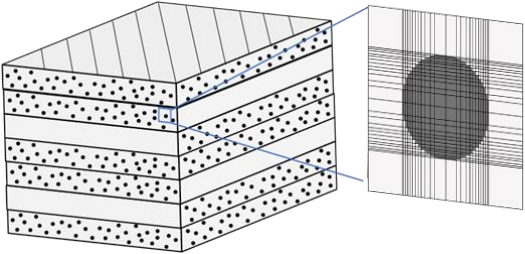
# ML Model Training



# LSTM Model

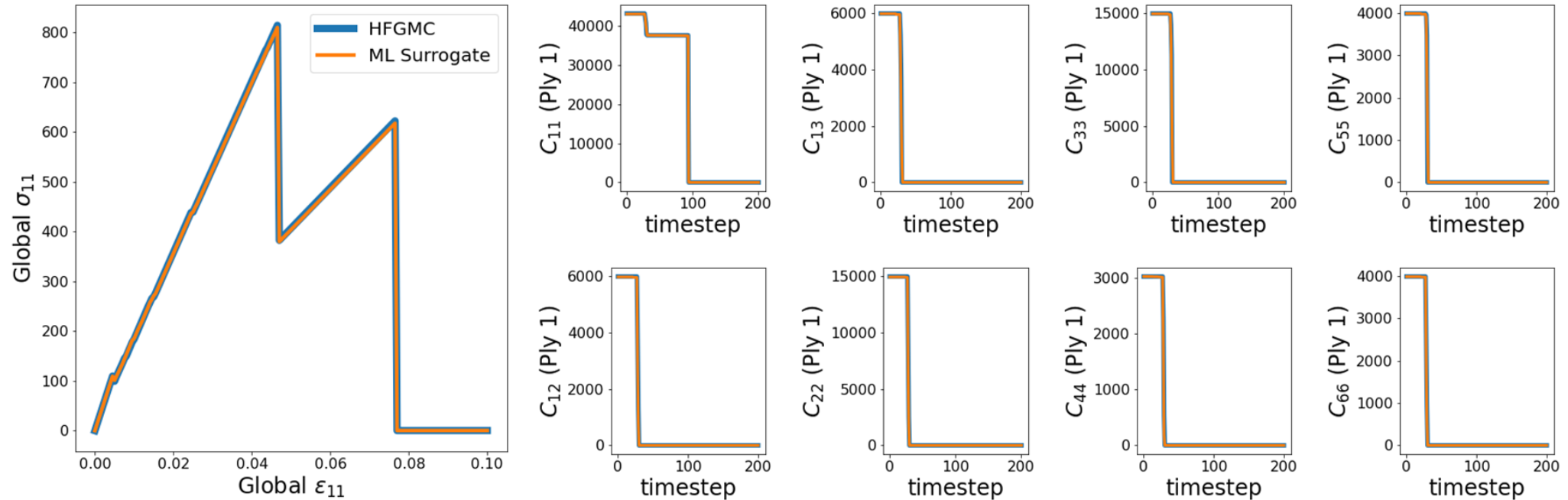


# LSTM Model Results

| Problem Configuration                                                                                            | Runtime (sec) |       |              |
|------------------------------------------------------------------------------------------------------------------|---------------|-------|--------------|
|                                                                                                                  | GMC           | HFGMC | ML Surrogate |
| 4 Ply<br>$2 \times 2$ RUC      | 14            | 14    | <b>3.5</b>   |
| 8 Ply<br>$2 \times 2$ RUC      | 17            | 18    | <b>5</b>     |
| 4 Ply<br>$26 \times 26$ RUC   | 326           | 442   | <b>3.5</b>   |
| 8 Ply<br>$26 \times 26$ RUC  | 605           | 827   | <b>5</b>     |

# LSTM Model Results

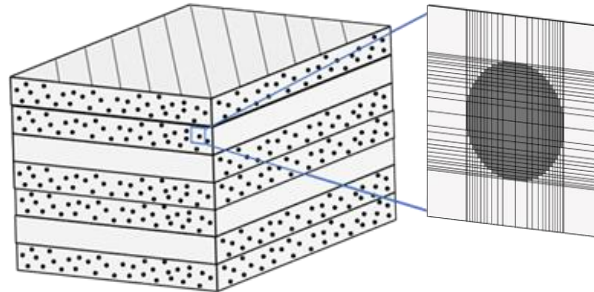
$26 \times 26$  RUC  $[0^\circ, 32.5^\circ, -32.5^\circ, 90^\circ, 90^\circ, -32.5^\circ, 32.5^\circ, 0^\circ]$



## Material Properties

|                         | Fiber     | Matrix |
|-------------------------|-----------|--------|
| <b>E</b>                | 75 GPa    | 4 GPa  |
| <b><math>\nu</math></b> | 0.25      | 0.35   |
| <b>UTS</b>              | 3,500 MPa | 60 MPa |

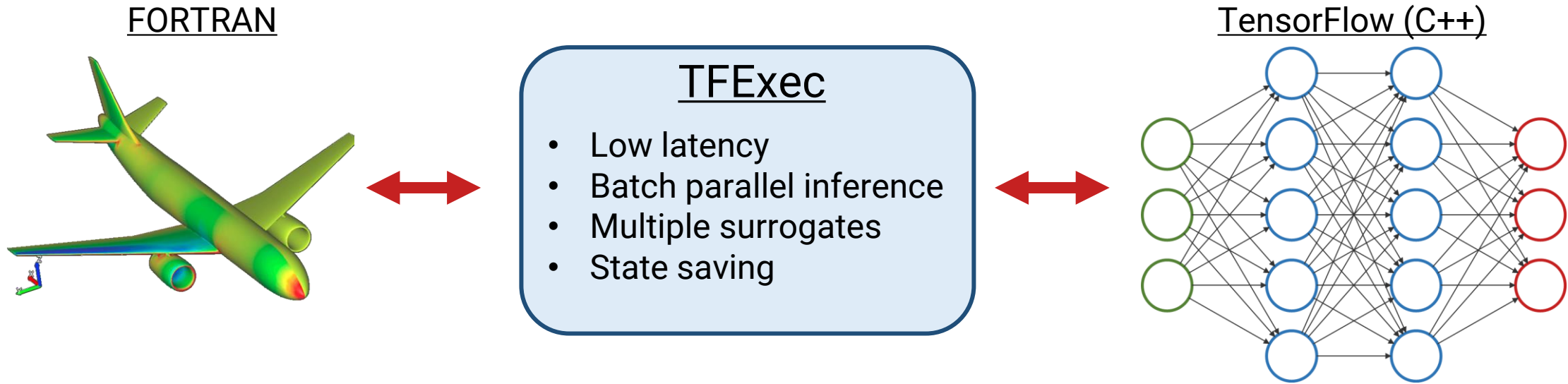
## Laminate Configuration



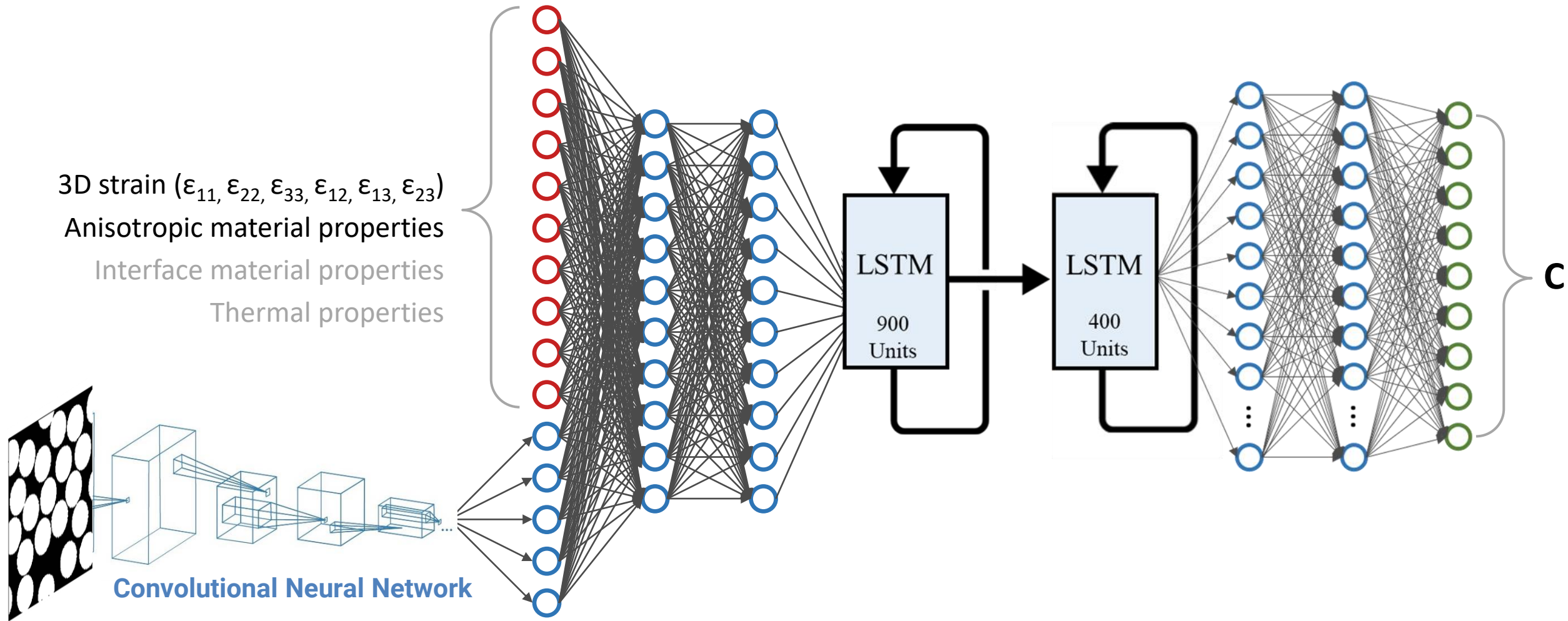
## Accuracy Results

|                      | MAE      | R <sup>2</sup> |
|----------------------|----------|----------------|
| <b>Global Stress</b> | 10.5 MPa | 0.98           |
| <b>Homogenized C</b> | 2.4 MPa  | 0.9997         |

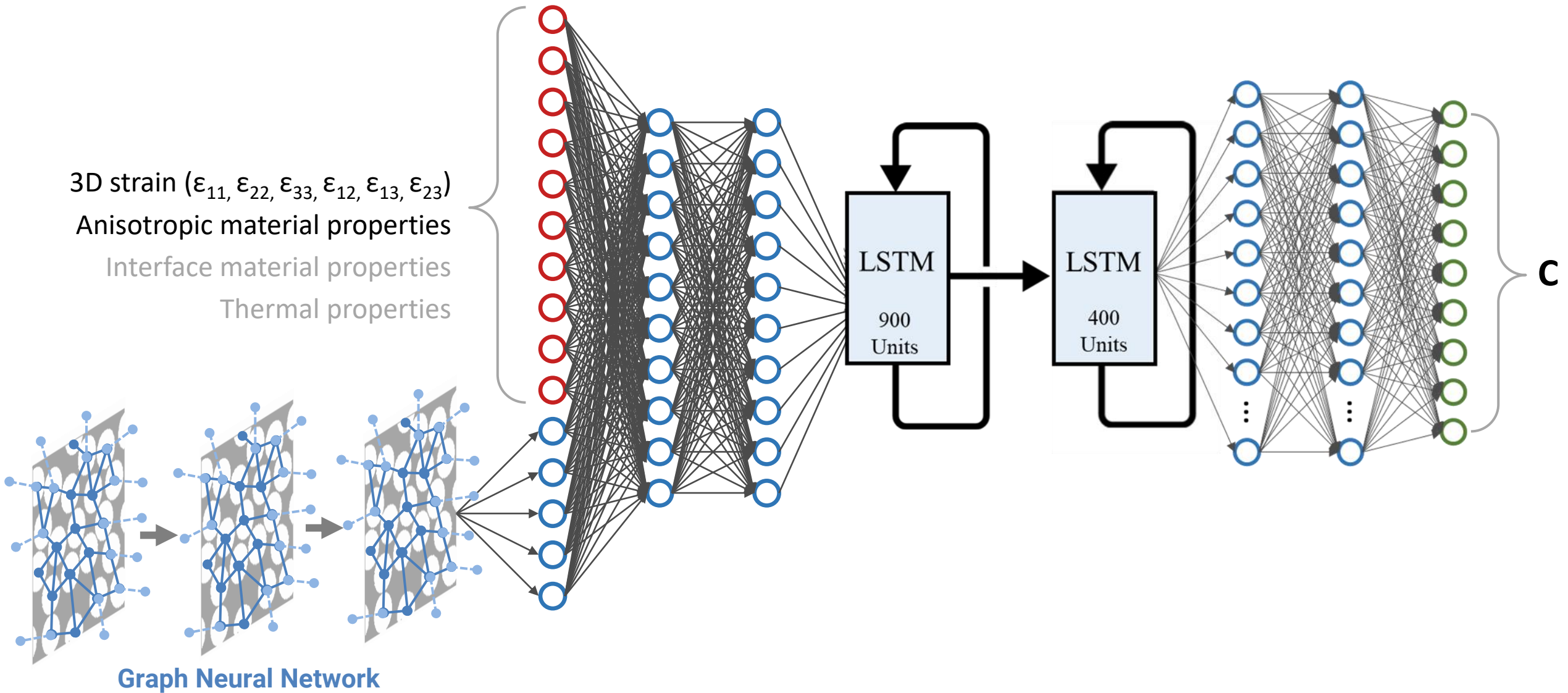
# ML/Physics Model Interfacing



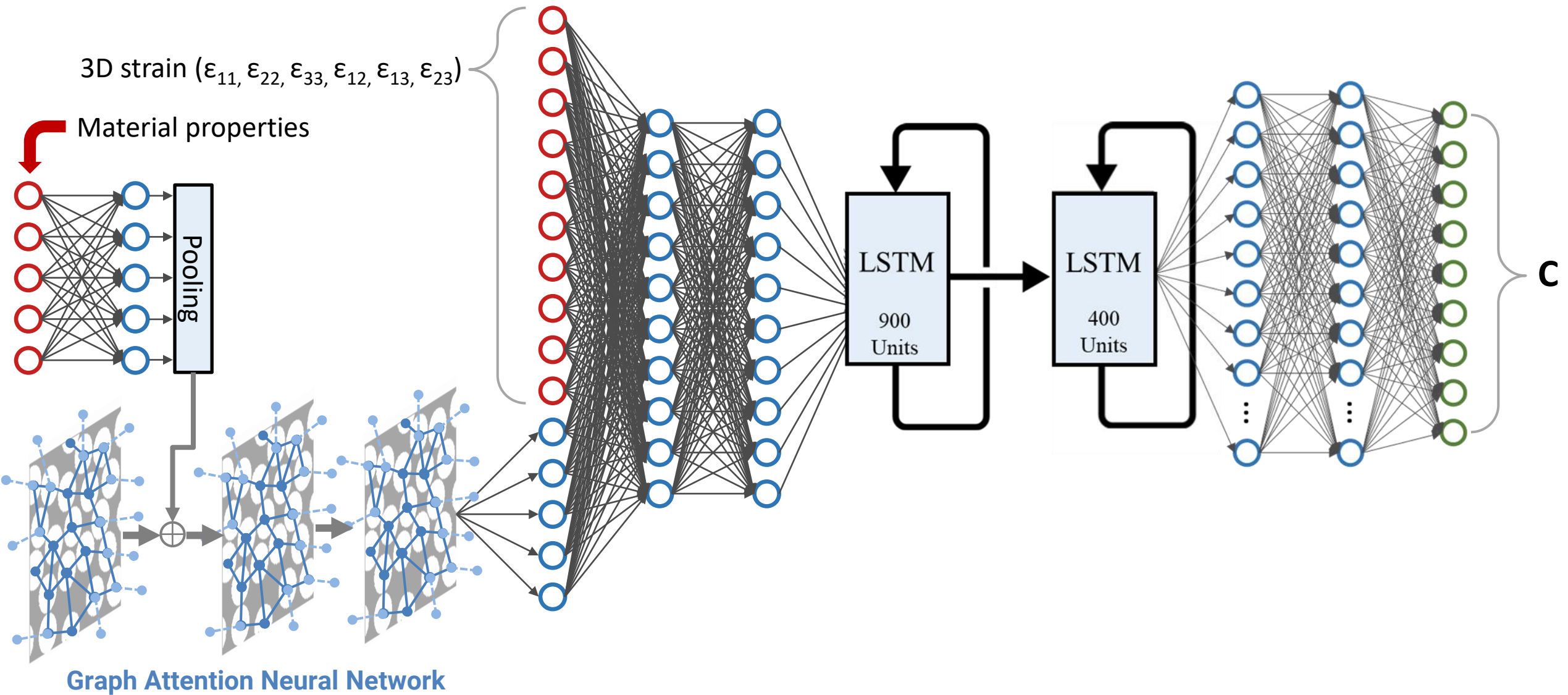
# Varying Microstructure



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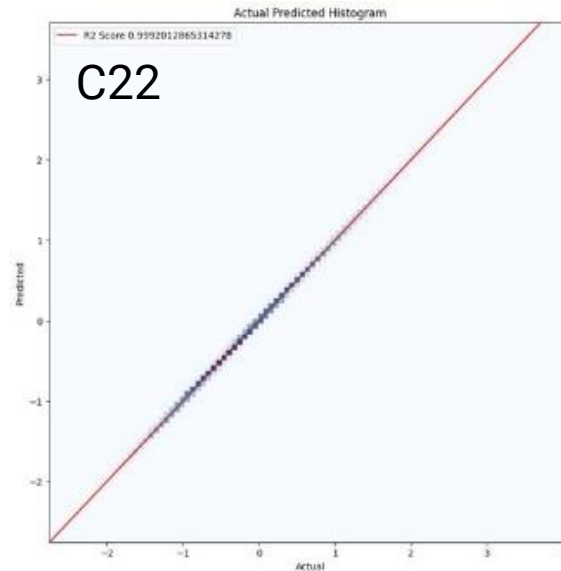
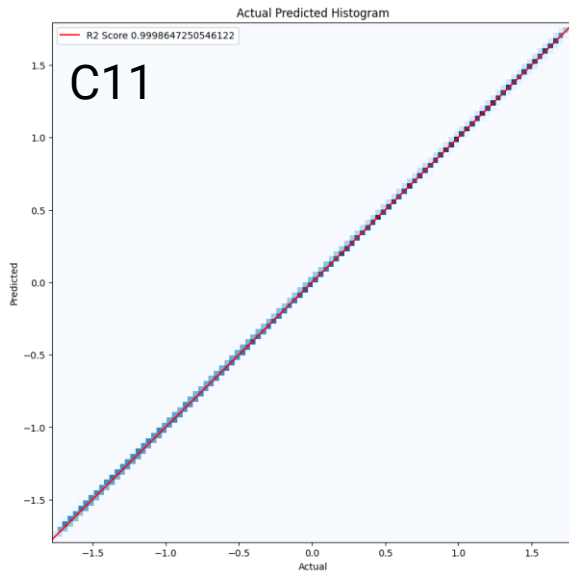
# Varying Microstructure



# GNN/LSTM Model Results

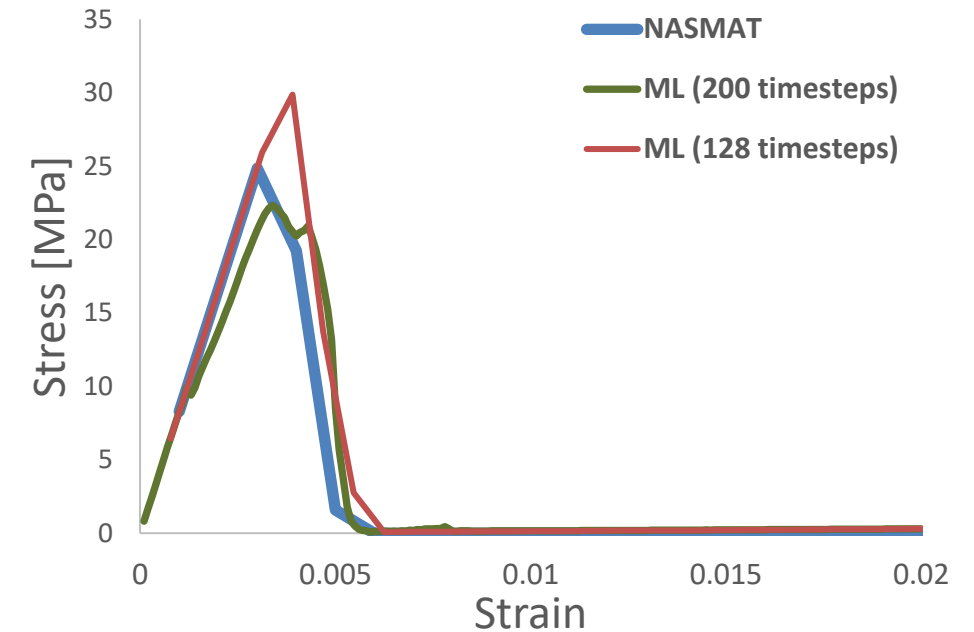
## Surrogate Model Accuracy:

**$r^2$ : 0.985 – 0.999** for each element of the stiffness tensor



## Combined multiscale model

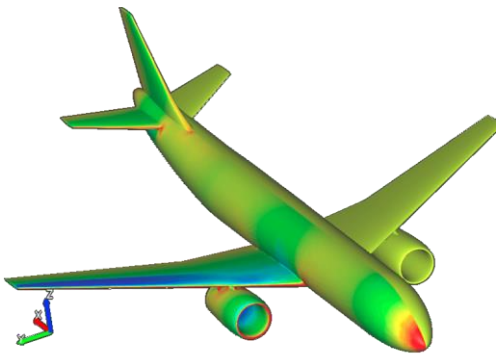
**MAE: 0.21 MPa** for stress predictions



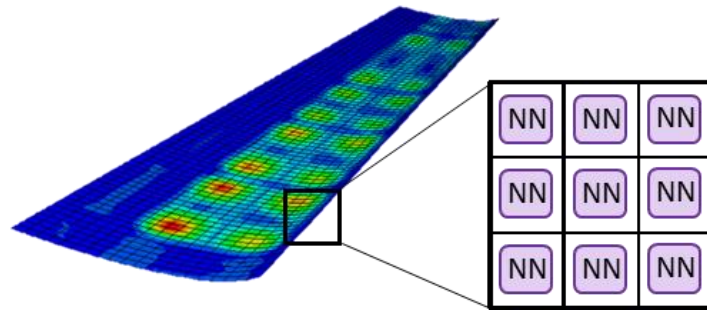
# Conclusions

Research level **accuracy** at commercially viable **speed**

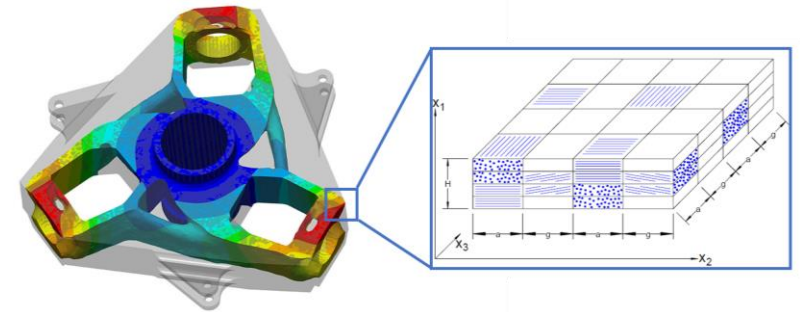
Targeting future applications



Design tools



Larger simulations



Optimization



# Thank you!

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