National Aeronautics and
Space Administration



Physics-Informed Deep Learning for Modeling & Simulation under Uncertainty

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Motivation

The future of air travel

New concepts, environments



New materials, fabrication

- Requires significant certification effort
- Can no longer rely on material databases built and adjusted through decades of experience
- Testing is expensive!

More complex materials, interfaces, etc.

+

New fabrication methods

= more uncertainty

Certification by Analysis (CBA)

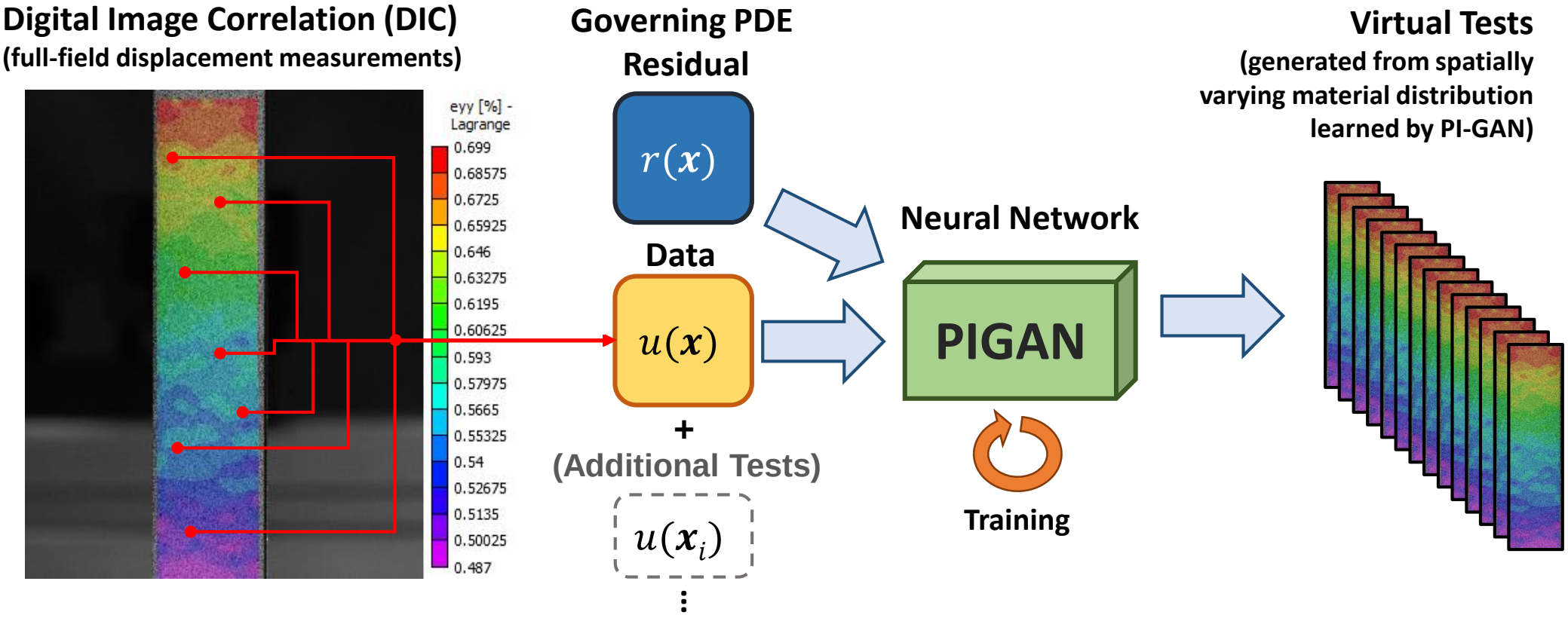
- Hardware testing is expensive and time-consuming
- Modeling and simulation can be used to supplement testing programs to reduce cost while maintaining or increasing reliability
- CBA typically requires:
  - High-fidelity simulations
  - Multi-scale modeling

  Development, verification and validation can be time consuming and expensive
  - Calibration using relatively small datasets ←Introduces additional uncertainty
  - Consideration of epistemic and aleatory uncertainties
    - Previously quantified through extensive testing programs
    - Uncertainty quantification (UQ) requires large number of repeated simulations
    - Can be intractable when using high-fidelity models

Deep Learning for CBA

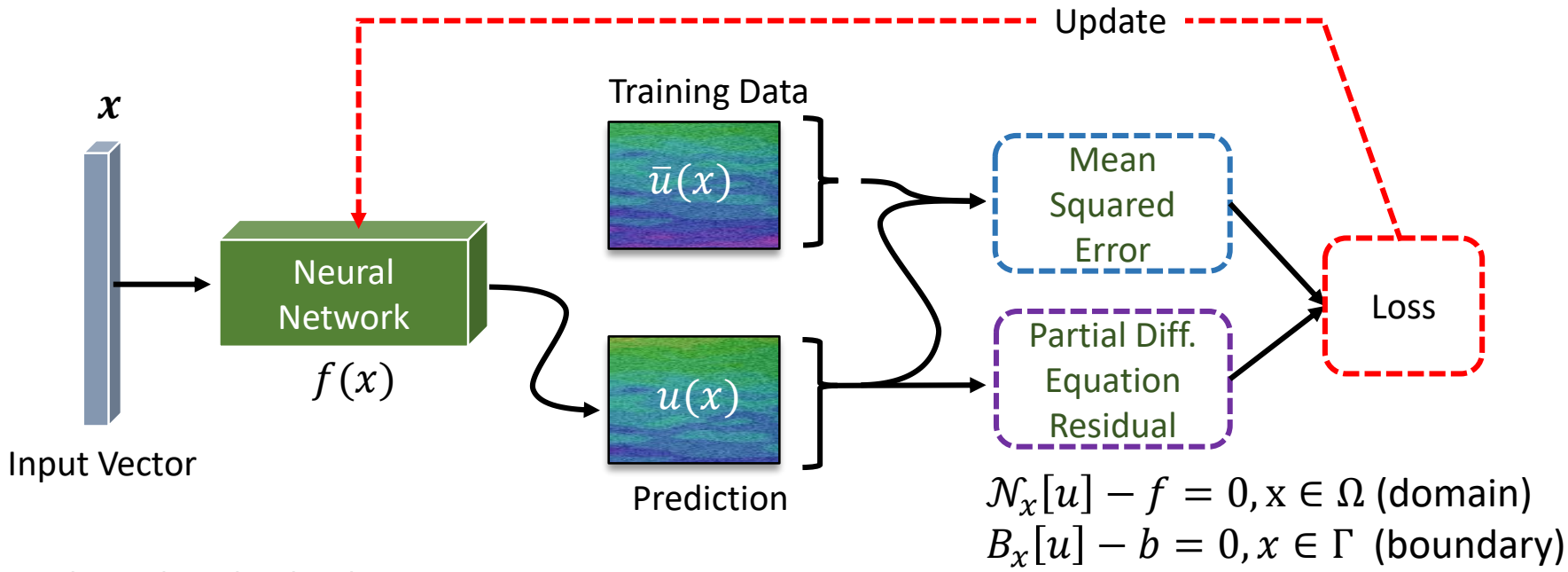
Material Identification and Generation using Artificial Intelligence

- Use a state-of-the-art artificial intelligence and deep learning concept – **Physics-Informed Generative Adversarial Networks (PIGANS)** – to develop a neural network (NN) capable of generating an infinite number of virtual material tests.



Background
Physics-informed Neural Networks (PINNs)

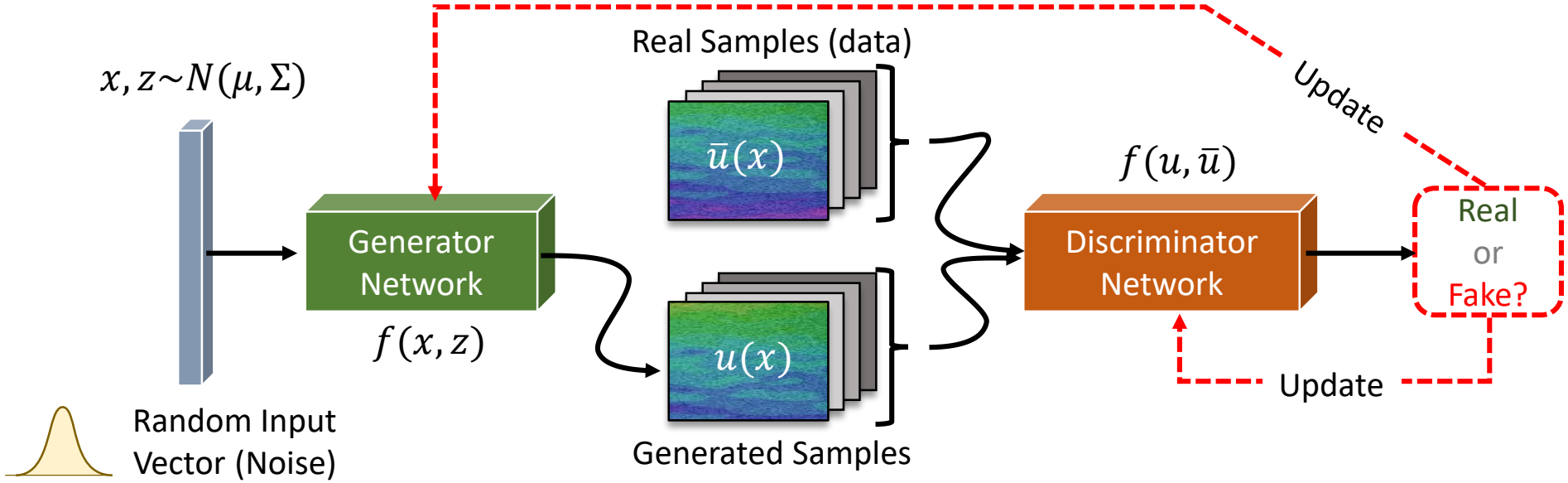
- Neural network trained to produce solution $u(x)$ to a partial differential equation
- Trained using two-part objective:
  1. Minimize mean squared error with respect to data
  2. Output physically admissible solutions throughout the problem domain



Raissi et al. "Physics-informed neural networks: A deep learning framework for solving forward and inverse..." *J. Comp. Phys.* (2019)

Background
Generative Adversarial Networks (GANs)

- Two neural networks compete in a zero-sum game
- Training objective: *discriminator network* tries to discern real from fake while *generator network* tries to fool the discriminator
- GANs are capable of learning/generating samples from complex probability distributions

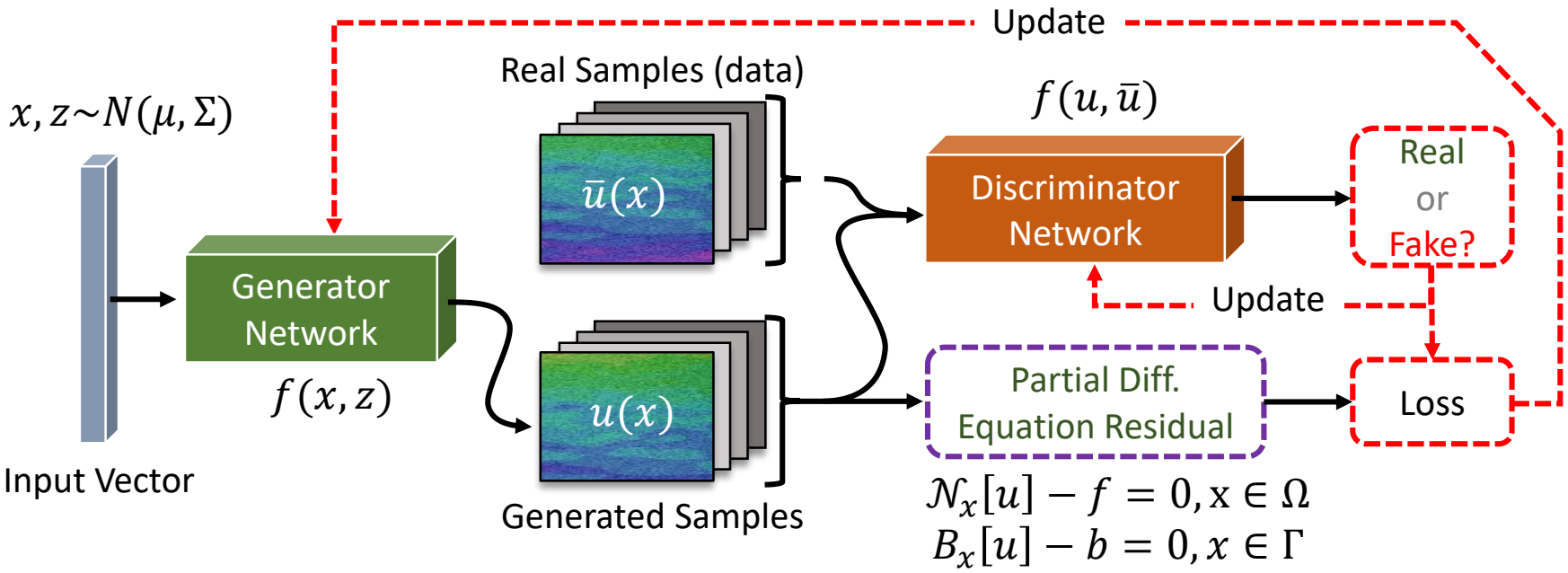


Goodfellow, Ian J., et al. "Generative adversarial networks." arXiv preprint arXiv:1406.2661 (2014)

Background

Physics-informed Generative Adversarial Networks (PIGANs)

- Combination of PINNs and GANs
- Enables learning of physically admissible, *probabilistic* solution, $\boldsymbol{u}(x)$

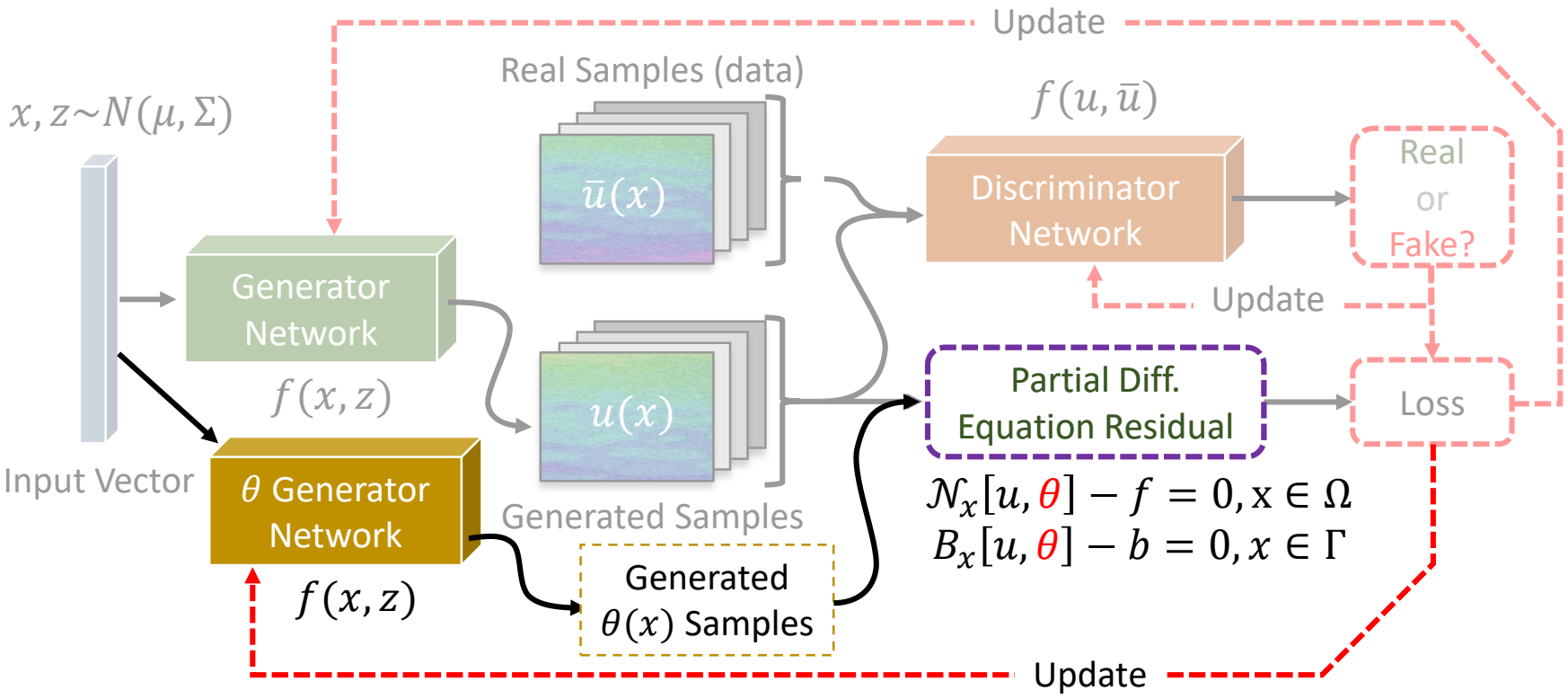


Yang et al. "Physics-informed generative adversarial networks for stochastic differential equations." arXiv preprint arXiv:1811.02033 (2018)

Background

Physics-informed Generative Adversarial Networks (PIGANs)

- Add generators for additional parameters, θ
- Enables solving complex, probabilistic inverse problems (no direct θ observations)

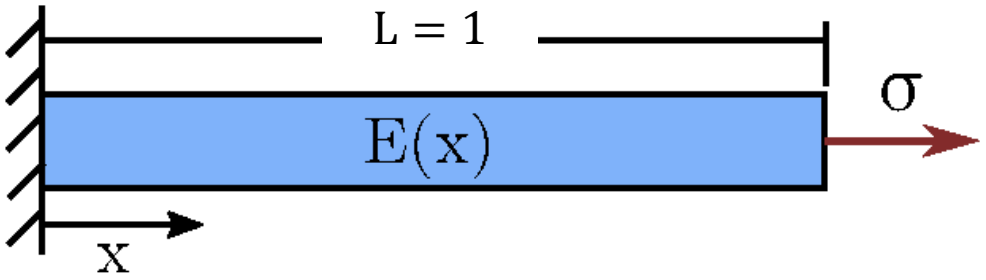


Yang et al. "Physics-informed generative adversarial networks for stochastic differential equations." arXiv preprint arXiv:1811.02033 (2018)

Application

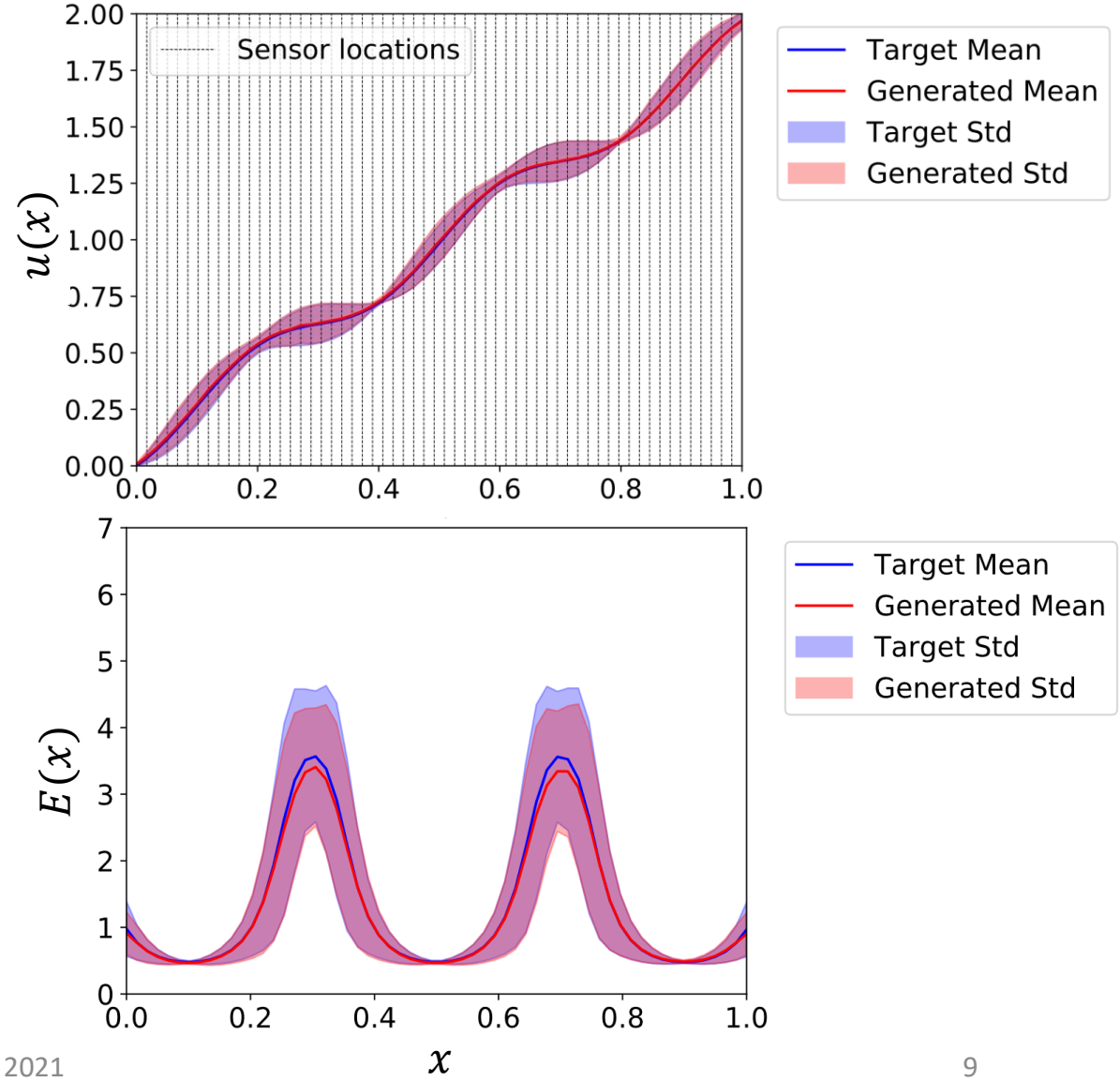
Example Problem: One-dimensional Bar in Tension

- 1D bar in tension with random, spatially-varying elastic modulus, $E(x)$
- Given measurements of displacement $u(x)$
- PIGAN learns material behavior and simultaneously quantifies uncertainty
  1. Learns the distribution $u(x)$ given 1,000 measurements at 60 sensors along bar
  2. Uses governing physics to inversely determine $E(x)$; i.e., no measurements of $E(x)$



$$E(x) = 1.2 + (sin(\frac{5\pi}{L}x + \frac{\pi}{2}(\beta - \frac{1}{2})))^{-1}$$

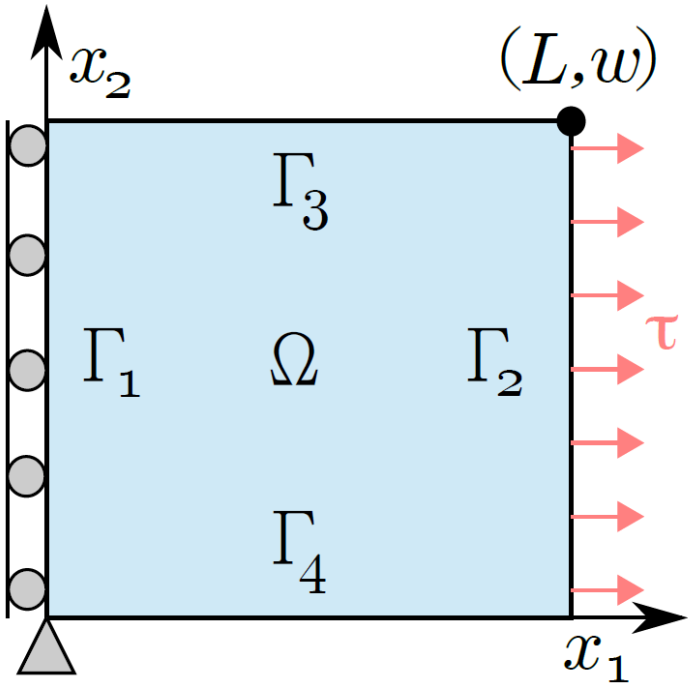
Random variable



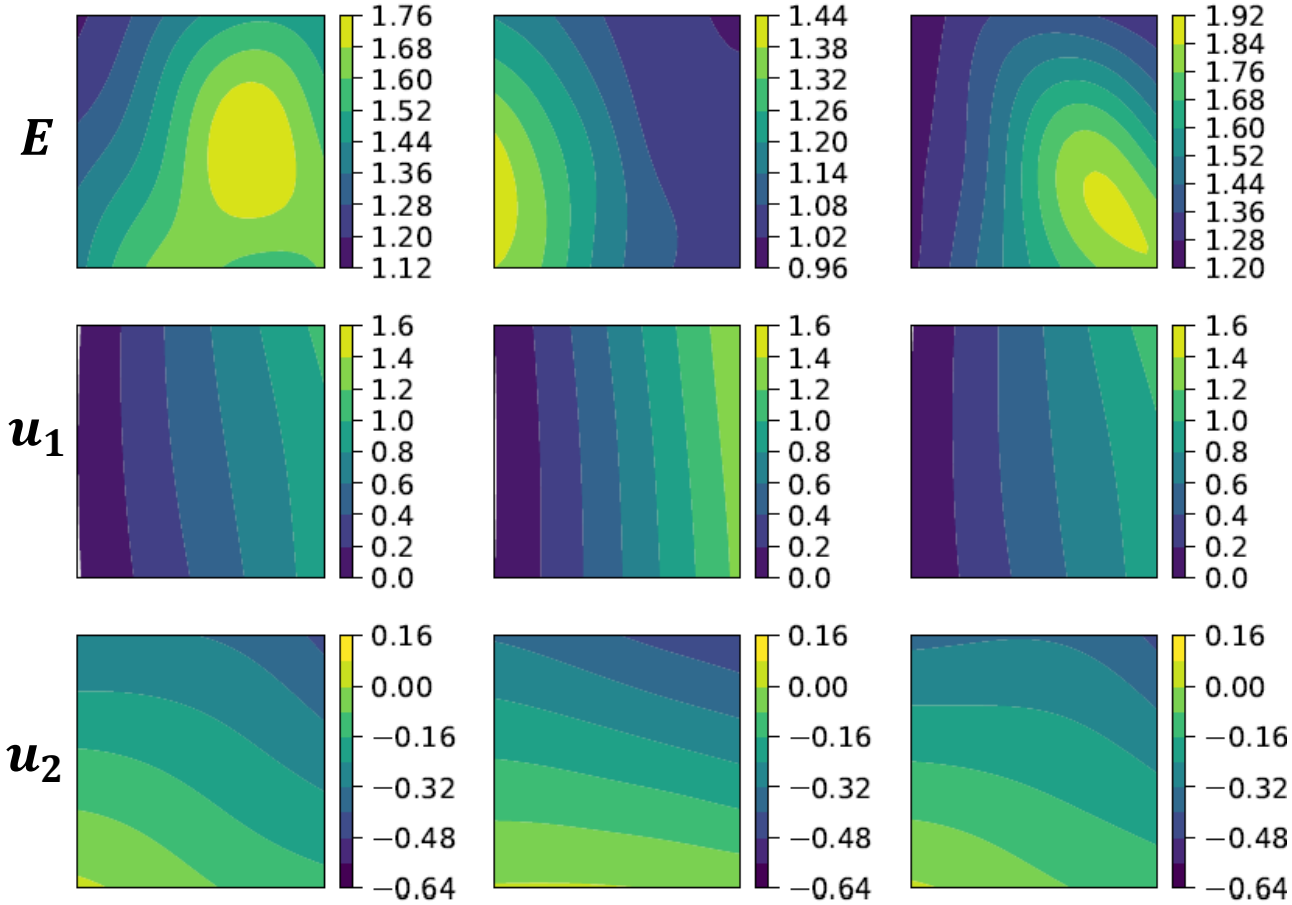
Application

Example Problem: Two-dimensional Plate in Tension

- 2D plate in tension with random, spatially-varying elastic modulus, $E(x)$
- Measurements of $\vec{u}(x)$ generated using Python finite element package FEniCS
- PIGAN learned both the $\vec{u}$ and E random fields

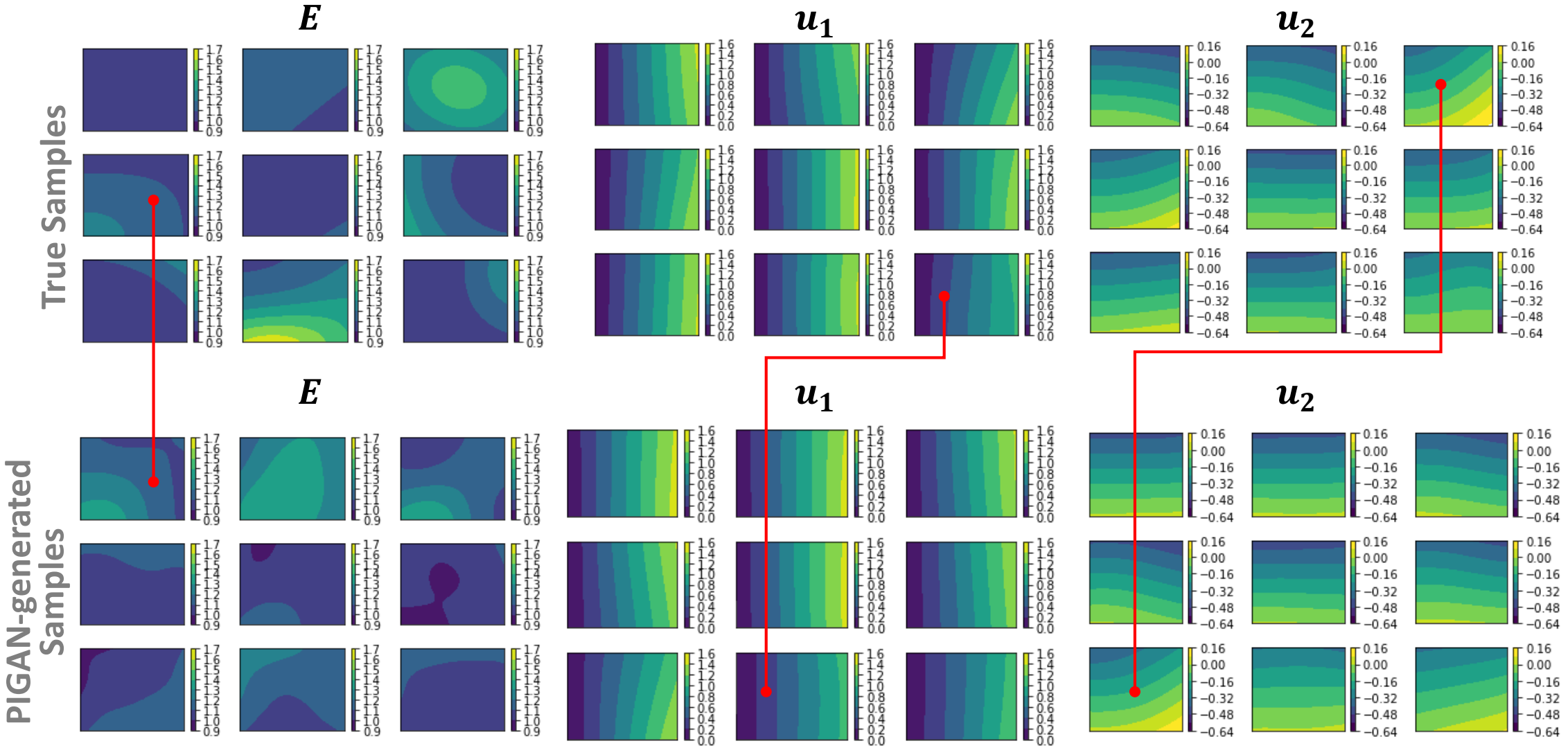


Randomly Generated Fields (Data Snapshots)



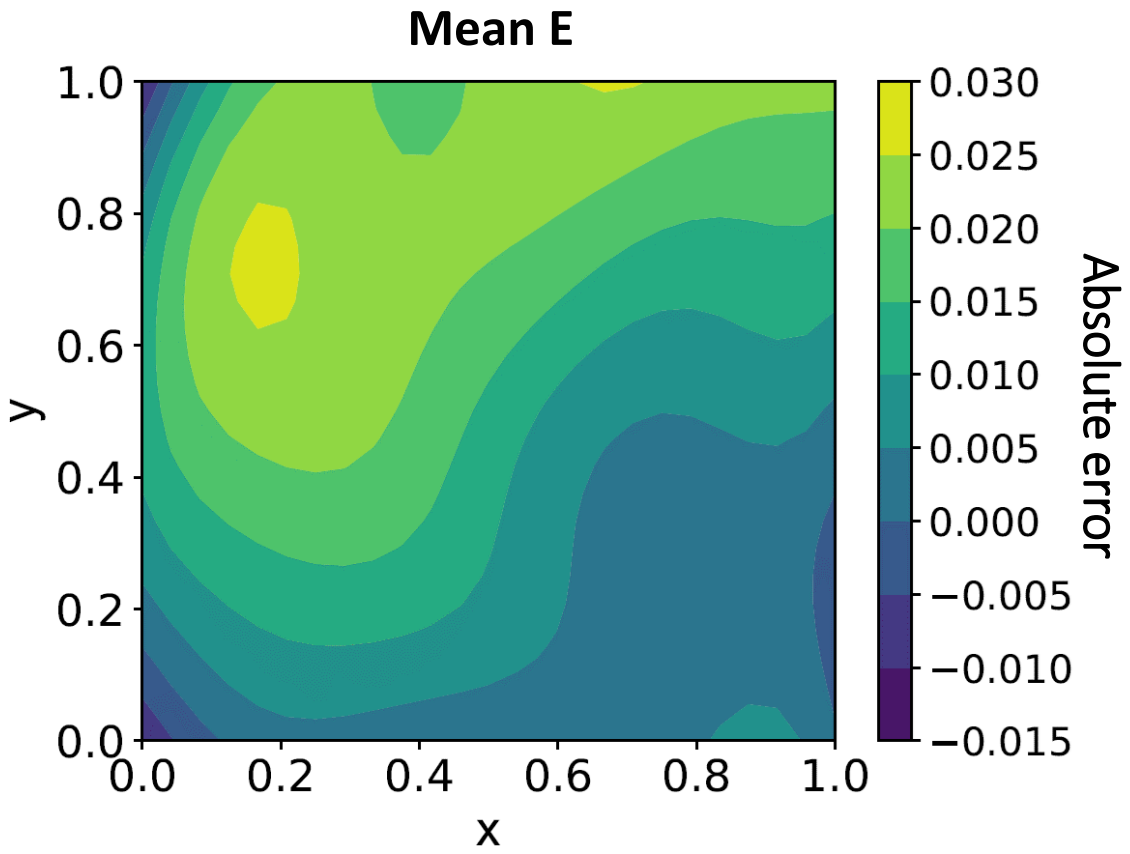
Application

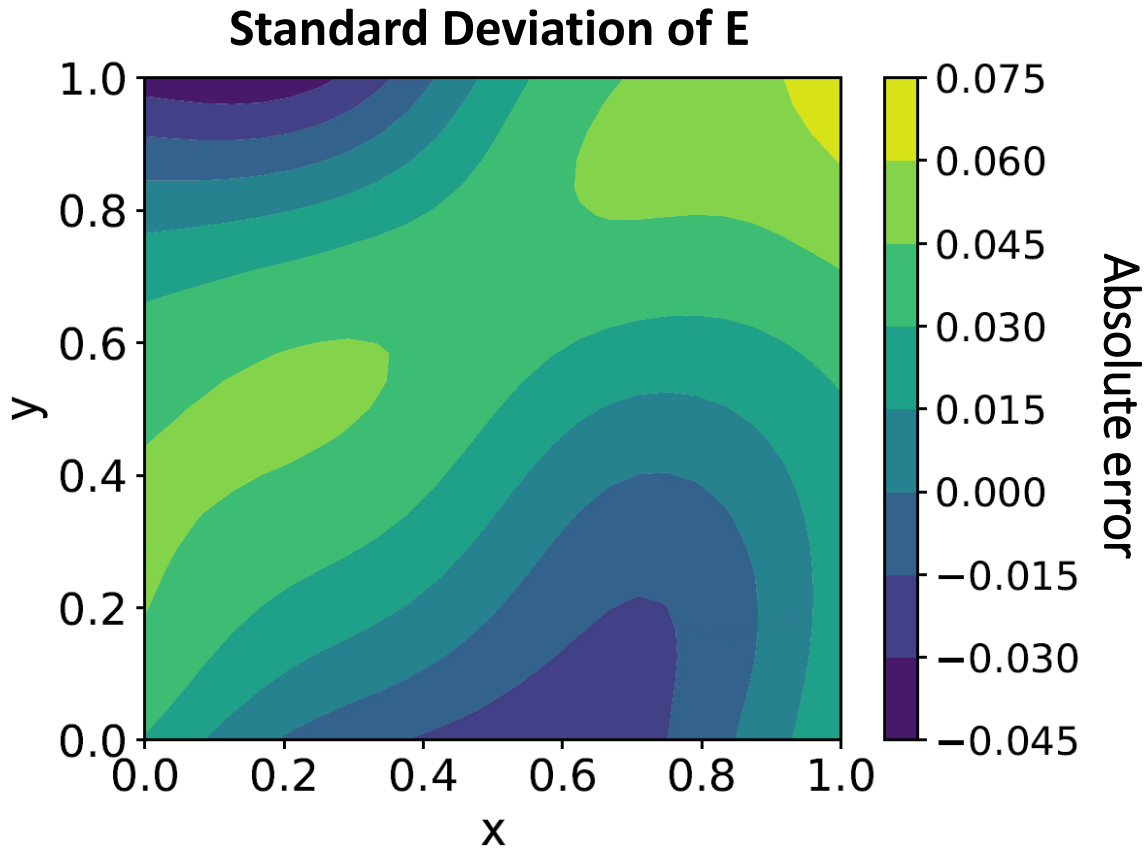
Example Problem: Two-dimensional Plate in Tension



Application

Example Problem: Two-dimensional Plate in Tension

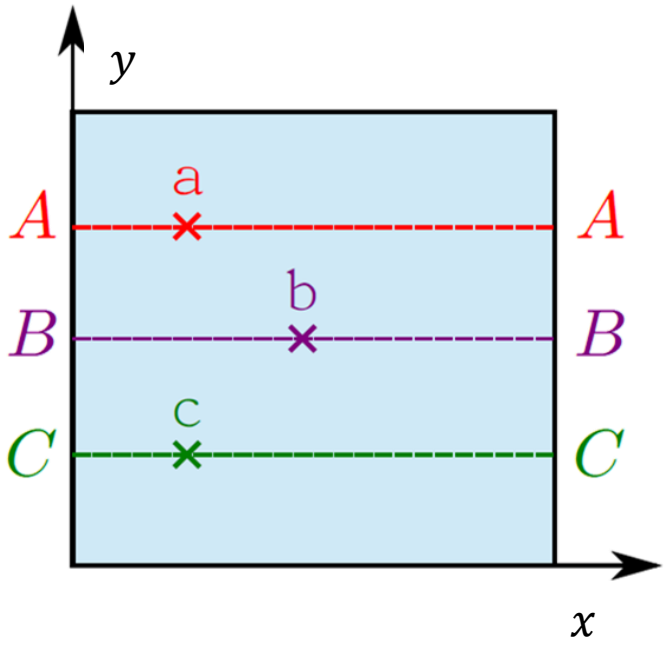




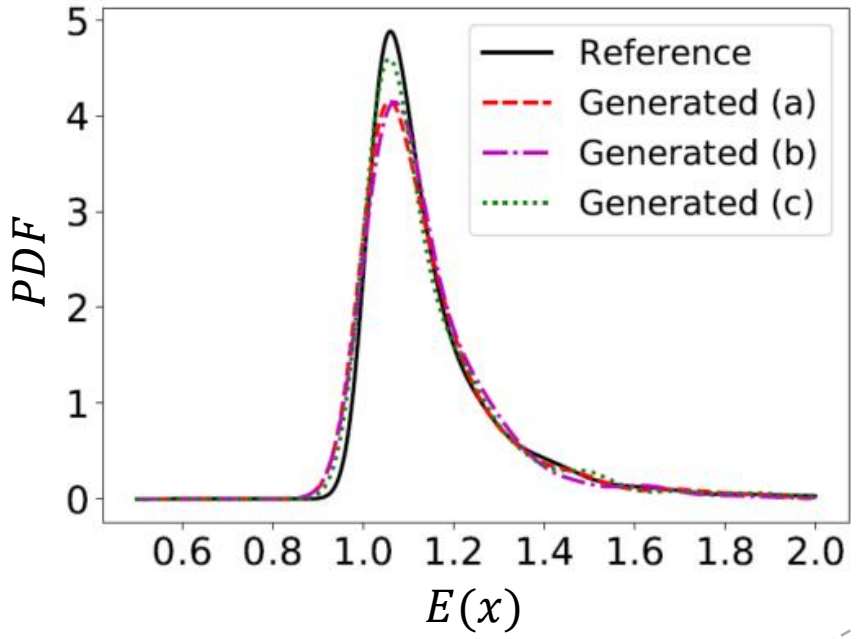
Note: magnitude of E is $\mathcal{O}(1)$

Application

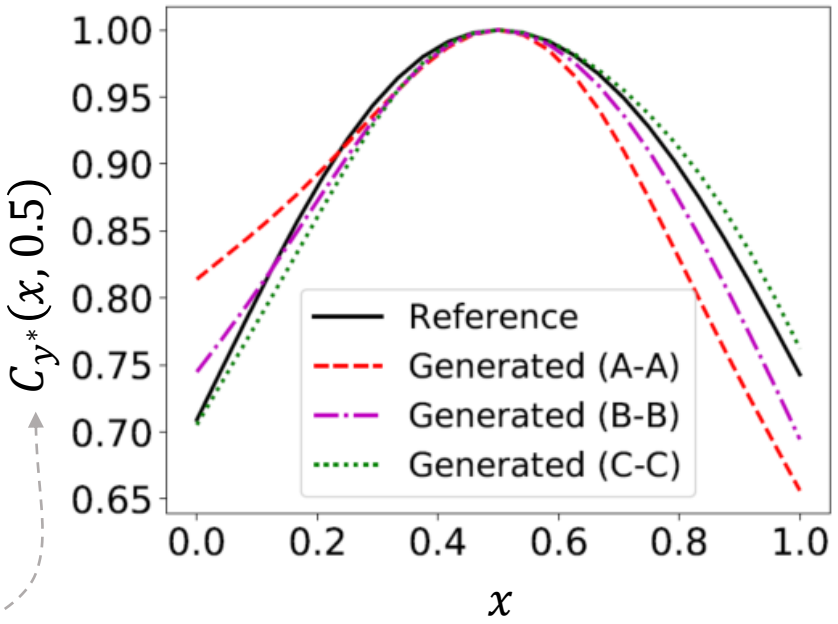
Example Problem: Two-dimensional Plate in Tension



Probability Density Function



Correlation Function



$$C_{y^*}(x, 0.5) = \text{Correlation}[E(x, y^*), E(0.5, y^*)]$$

Practical Considerations
Computational Expense

- Conducted speed study on the 1D bar example problem
- Conclusion: hardware is important

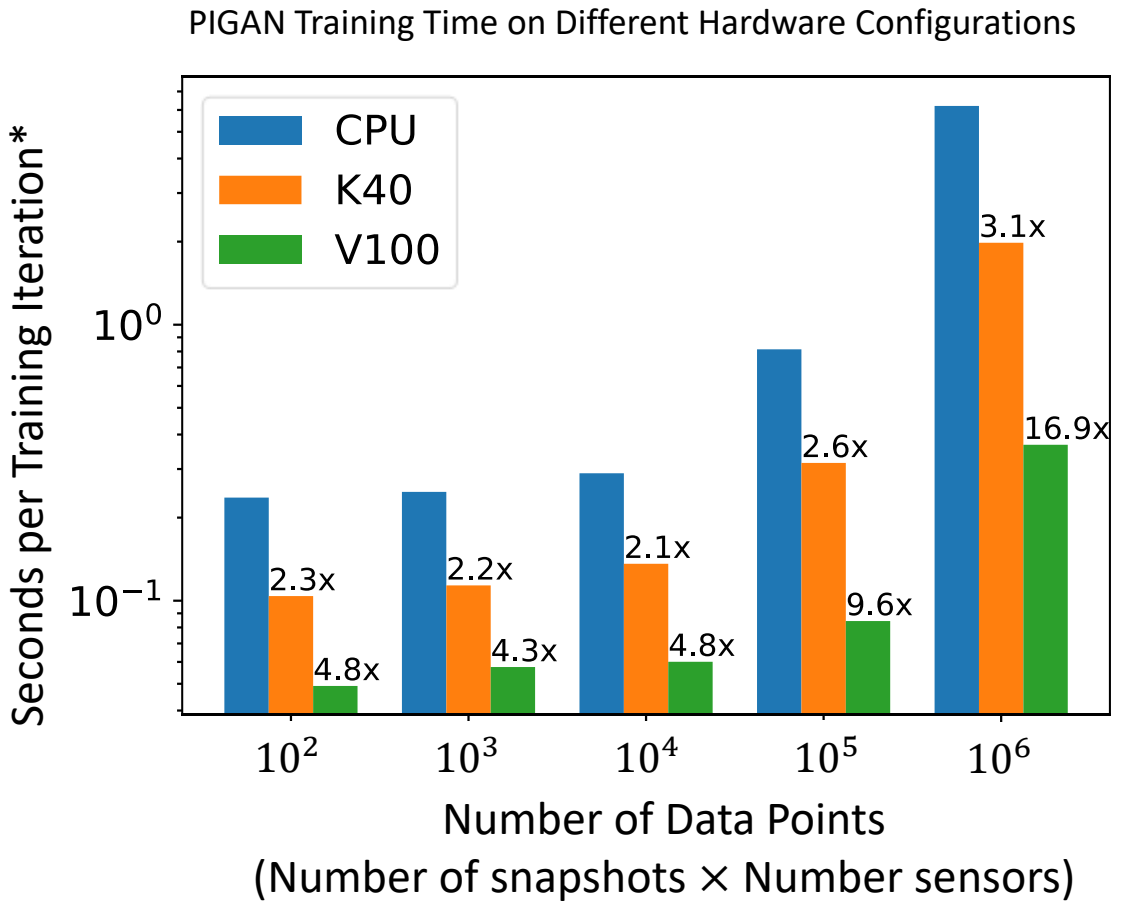
Central Processing Unit (CPU):

- Dual socket 8 core 2.60 GHz Intel E5-2640v3 Haswell Node

Graphics Processing Units (GPUs):

- NVIDIA Tesla K40
- NVIDIA Tesla V100

**All tests run on LaRC midrange K-Cluster*



*Number of training iterations typically on the order of $10^4 - 10^5$ for examples shown in this presentation

Practical Considerations

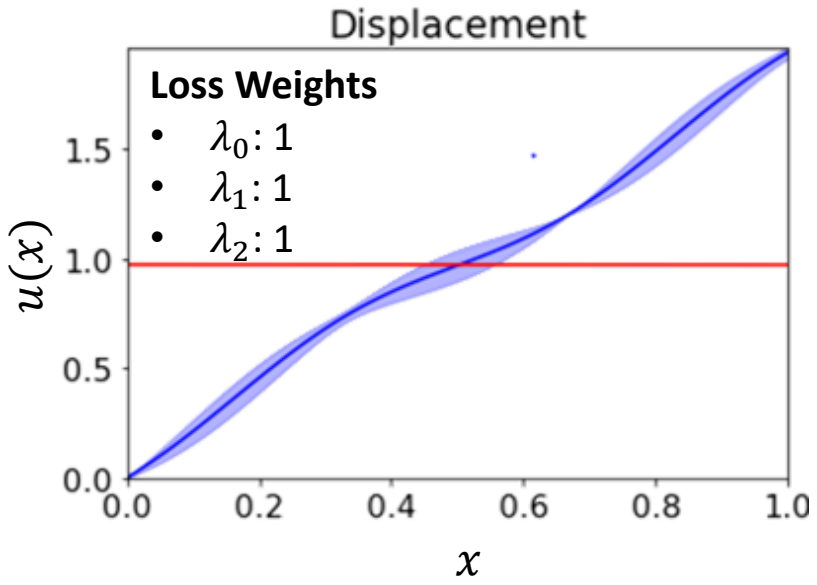
Addressing Training Instabilities in the 1D and 2D Examples

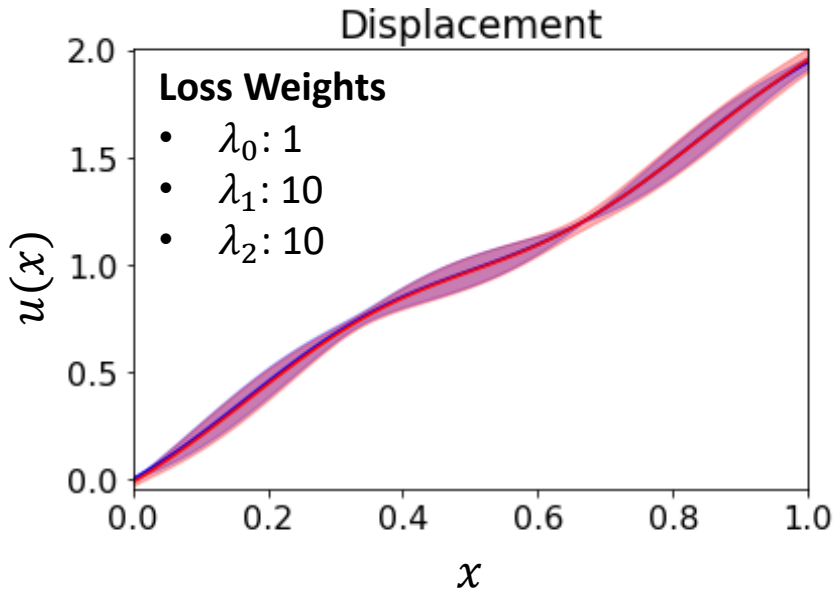
- When training, goal is to minimize a loss function
- Example:

PDE inside domain *Boundary conditions*

$$L_{Gen}^{PIGAN} = L_{Gen}^{GAN} + \lambda_0 L_\Omega + \lambda_1 L_{\Gamma 1} + \lambda_2 L_{\Gamma 2} + \lambda_3 L_{\Gamma 3} + \lambda_4 L_{\Gamma 4} + \lambda_5 L_{\Gamma 5} + \lambda_6 L_{\Gamma 6} \ldots$$

- Loss function imbalance can cause training instabilities and poor predictive capability





Practical Considerations

Addressing Training Instabilities in the 1D and 2D Examples

- When training, goal is to minimize a loss function
- Example:

PDE inside domain *Boundary conditions*

$$L_{Gen}^{PIGAN} = L_{Gen}^{GAN} + \lambda_0 L_{\Omega} + \lambda_1 L_{\Gamma 1} + \lambda_2 L_{\Gamma 2} + \lambda_3 L_{\Gamma 3} + \lambda_4 L_{\Gamma 4} + \lambda_5 L_{\Gamma 5} + \lambda_6 L_{\Gamma 6} \ldots$$

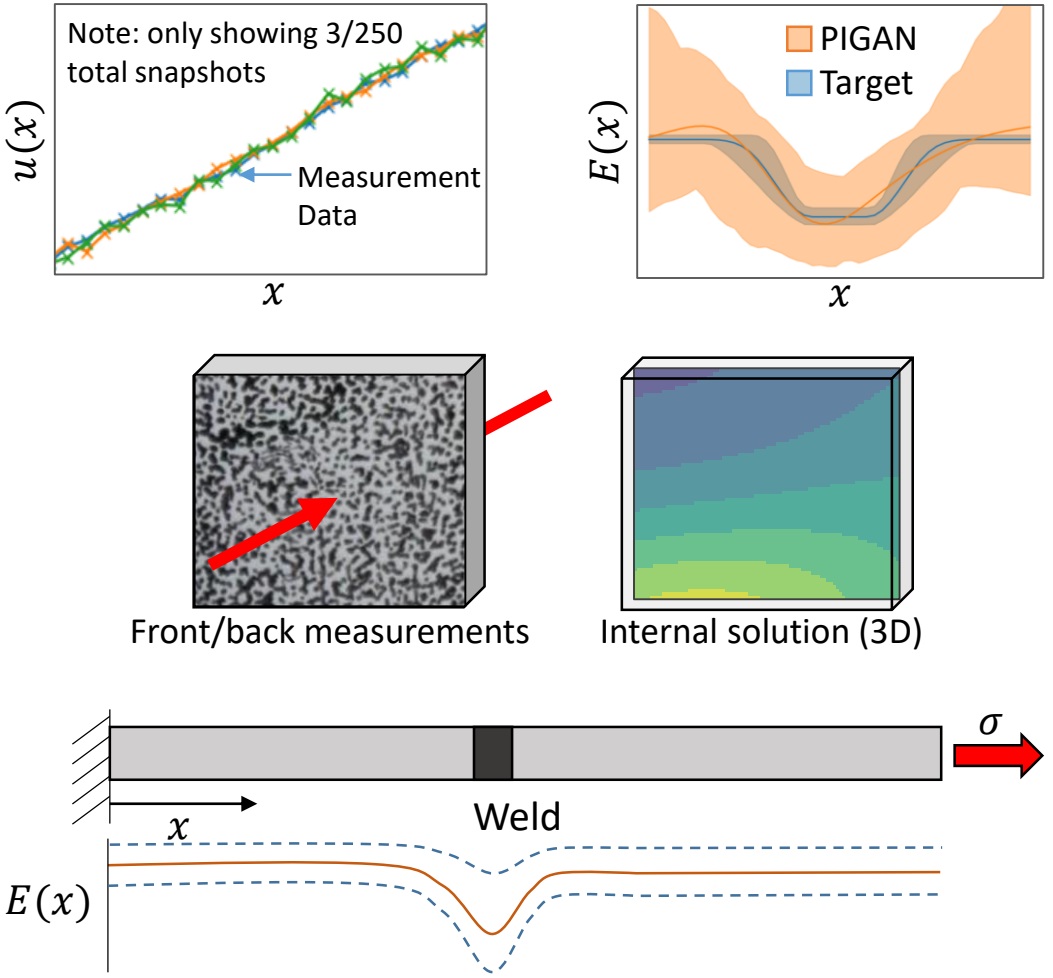
- Loss function imbalance can cause training instabilities and poor predictive capability
- Found that relative balance between L_{Gen}^{PIGAN} and $L_{Disc}^{PIGAN} = L_{Disc}^{GAN}$ was more important than individual weights (λ_i)
  - Tuning this balance through nested training drastically improved success rates (e.g., 5 updates of generator for every update of the discriminator)
  - Appears to be *problem dependent*
  - Active area of research:

1. Wang et al. "Understanding and mitigating gradient pathologies in physics-informed neural networks." arXiv preprint arXiv:2001.04536 (2020).
2. Wang et al. "When and why PINNs fail to train: A neural tangent kernel perspective." arXiv preprint arXiv:2007.14527 (2020).

Moving Forward

Current Areas of Focus

- Training PIGANs in the presence of measurement noise
- Solving for three-dimensional displacement/property fields
- Increasing application realism and relevance to NASA



Summary

- Introduced **Physics-informed Generative Adversarial Networks (PIGANs)** as a potential tool for certification by analysis
- Demonstrated probabilistic material identification capability on two examples
  - 1) 1D bar in tension and 2) 2D plate in tension
  - Both examples involved a random, spatially-varying elastic modulus
- Preprint available online:
  - Warner, James E., et al. "Inverse Estimation of Elastic Modulus Using Physics-Informed Generative Adversarial Networks." *arXiv:2006.05791* (2020).
- Contact information: patrick.e.leser@nasa.gov