Physics-Informed Loss Functions

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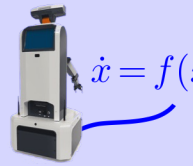
Physics-Informed Loss

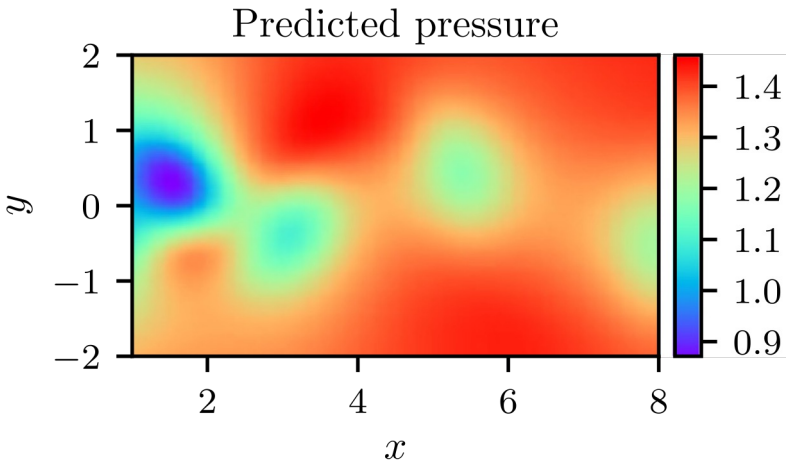
$$\mathcal{L} = \mathcal{L}_{\text{physics}} + \mathcal{L}_{\text{data}}$$

bound. cond.
$||x(0) - x_0||^2$

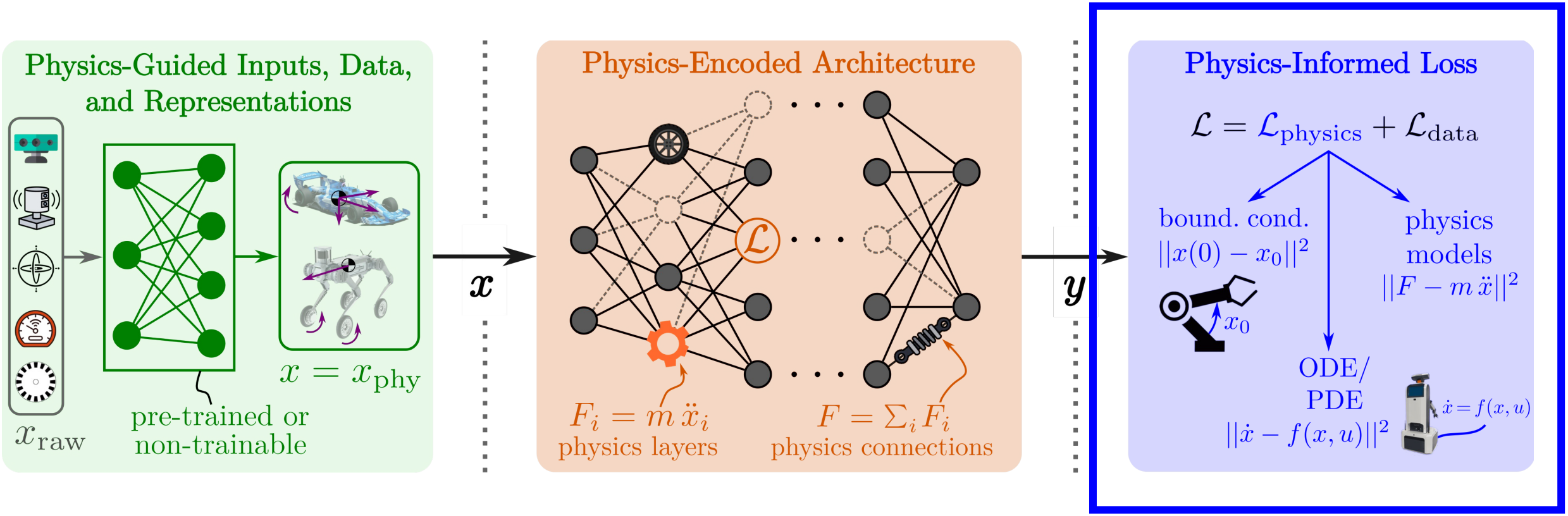
physics models
$||F - m\,\ddot{x}||^2$

ODE/ PDE
$||\dot{x} - f(x,u)||^2$





Physics-Informed Learning: Positioning

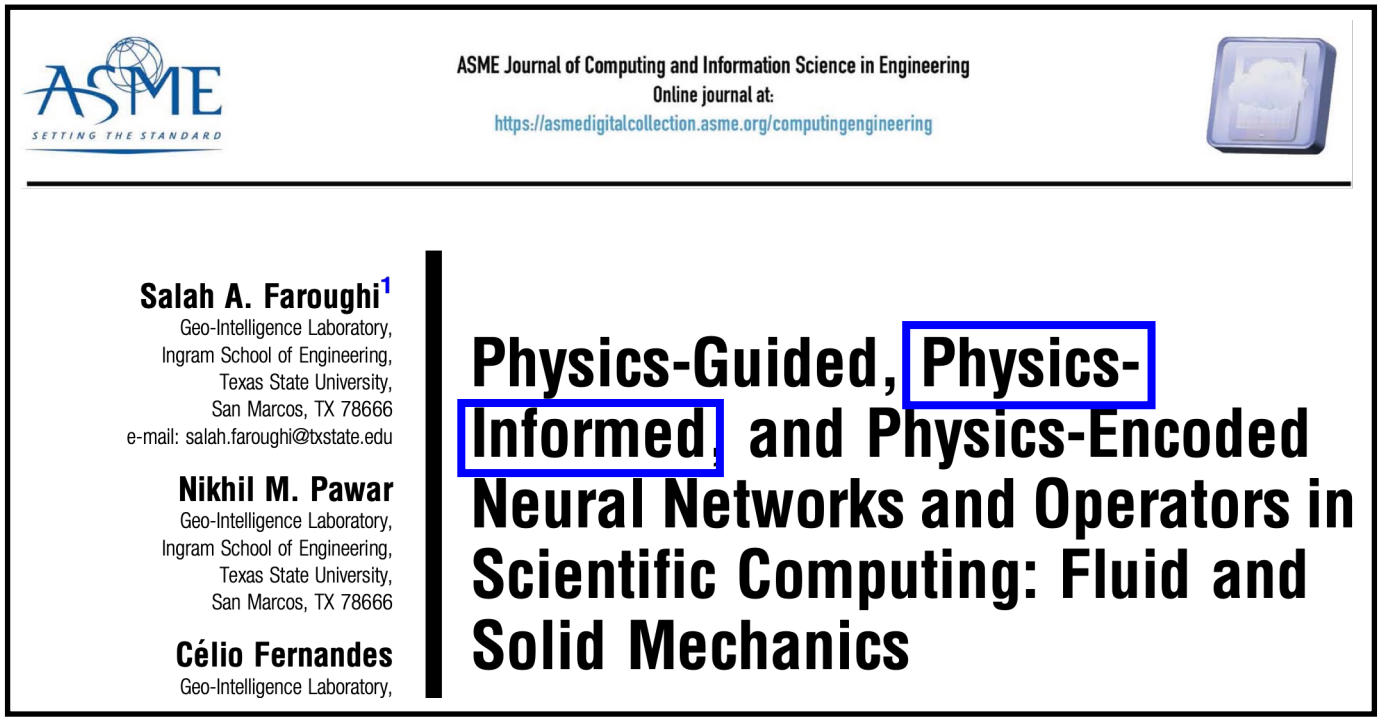


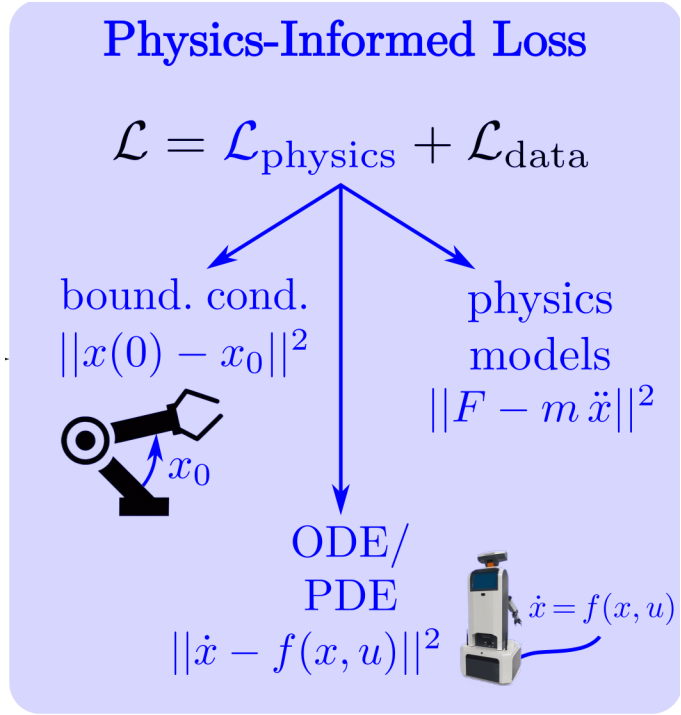
What Is Physics-Informed Learning?

Governing **physical equations** imposed as ***soft constraints*** in the **loss function**

1. Learn the **solutions** of hard-to-solve physical equations
2. Improve accuracy of imperfect physical models through **physics + data loss**

Better generalization in **data-scarse regimes**, compared to purely data-driven NNs





Physics-Informed Learning: Seminal Paper

Neural Networks to ***solve*** or ***discover*** **Partial Differential Equations** (PDEs)

Nonlinear **PDE**: $u_t + \mathcal{N}[u; \lambda] = 0$

$u(t, x) =$ unknown solution, $u_t = \frac{\partial u(t,x)}{\partial t}$, λ = known or unknown parameters,
$\mathcal{N}[u; \lambda] =$ nonlinear operator

Includes physical PDEs for diffusion processes, fluid dynamics, … and ODEs!

Question 1: given λ, can a NN learn the solution $u(t, x)$?

Question 2: what is the best λ to fit observed data? → „discovery“ of PDEs

M. Raissi, P. Perdikaris, G.E. Karniadakis, “Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations”, *Journal of Computational Physics*, 2018

Neural Networks to Solve Partial Differential Equations

$$u_t + \mathcal{N}[u;\lambda] = 0 \quad \Longrightarrow \quad f := u_t + \mathcal{N}[u]$$

Learn the unknown $u(t,x)$ with a Neural Network (NN)

Loss function for NN training: $MSE = MSE_u + MSE_f$ (MSE = Mean Square Error)

$$MSE_u = \frac{1}{N_u}\sum_{i=1}^{N_u} |u(t_u^i, x_u^i) - u^i|^2 \quad \Longrightarrow \quad \text{Initial and } \textbf{boundary conditions} \text{ (known)}$$

$$MSE_f = \frac{1}{N_f}\sum_{i=1}^{N_f} |f(t_f^i, x_f^i)|^2 \quad \Longrightarrow \quad \textbf{Penalize violations} \text{ of the governing } \textbf{PDE}$$

Commonly known as **Physics-Informed Neural Networks** (**PINNs**)

M. Raissi, P. Perdikaris, G.E. Karniadakis, "Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations", *Journal of Computational Physics*, 2018

Neural Networks to Solve Partial Differential Equations

$$u_t + \mathcal{N}[u; \lambda] = 0$$

Remarks:

- $u(t, x)$ is a **general-purpose NN** (no physics in the architecture!)
- **No theoretical guarantee** to find the exact solution of the PDE
- **In practise**: If the PDE is well-posed and its solution is unique, a sufficiently deep NN will approximate the solution with good accuracy
- Once trained, PINN evaluation is **way faster** than PDE numerical solvers

Extended approach: combine **data + physics *regularization* loss** to improve generalization of NNs in data-scarce operation

$$\mathcal{L} = \mathcal{L}_{data} + \mathcal{L}_{physics}$$

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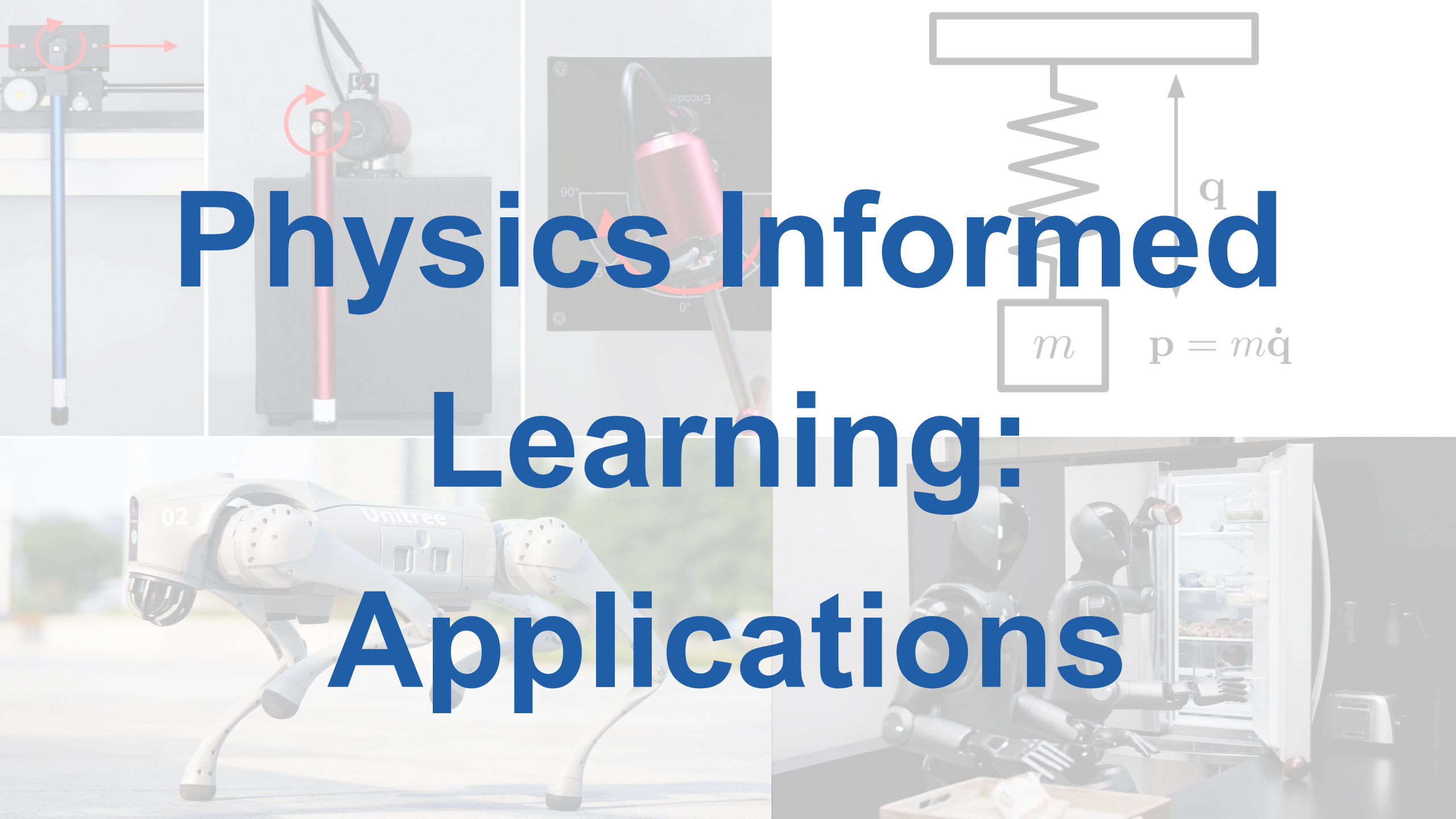
Questions & Discussion



Physics Informed Learning: Applications

Physics-Informed Neural Networks (PINNs) - Examples

Learn solutions of the **Schrödinger equation** (wave propagation)

$$ih_t + 0.5h_{xx} + |h|^2 h = 0, \quad x \in [-5, 5], \quad t \in [0, \pi/2],$$

$$h(0, x) = 2\,\mathrm{sech}(x),$$

$$h(t, -5) = h(t, 5),$$

$$h_x(t, -5) = h_x(t, 5),$$

$$\rightarrow \quad f := ih_t + 0.5h_{xx} + |h|^2 h$$

- **Nonlinear PDE** with **periodic** boundary conditions
- $h(t, x) = [u(t, x) \;\; v(t, x)]$ is a **complex-valued** solution
- $h(t, x)$ is learned with a 5-layer **NN**

Loss function: $MSE = MSE_0 + MSE_b + MSE_f$

Initial condition: $$MSE_0 = \frac{1}{N_0} \sum_{i=1}^{N_0} |h(0, x_0^i) - h_0^i|^2$$

Schrödinger eq.: $$MSE_f = \frac{1}{N_f} \sum_{i=1}^{N_f} |f(t_f^i, x_f^i)|^2$$

Periodic B.C.: $$MSE_b = \frac{1}{N_b} \sum_{i=1}^{N_b} \left(|h^i(t_b^i, -5) - h^i(t_b^i, 5)|^2 + |h_x^i(t_b^i, -5) - h_x^i(t_b^i, 5)|^2 \right)$$

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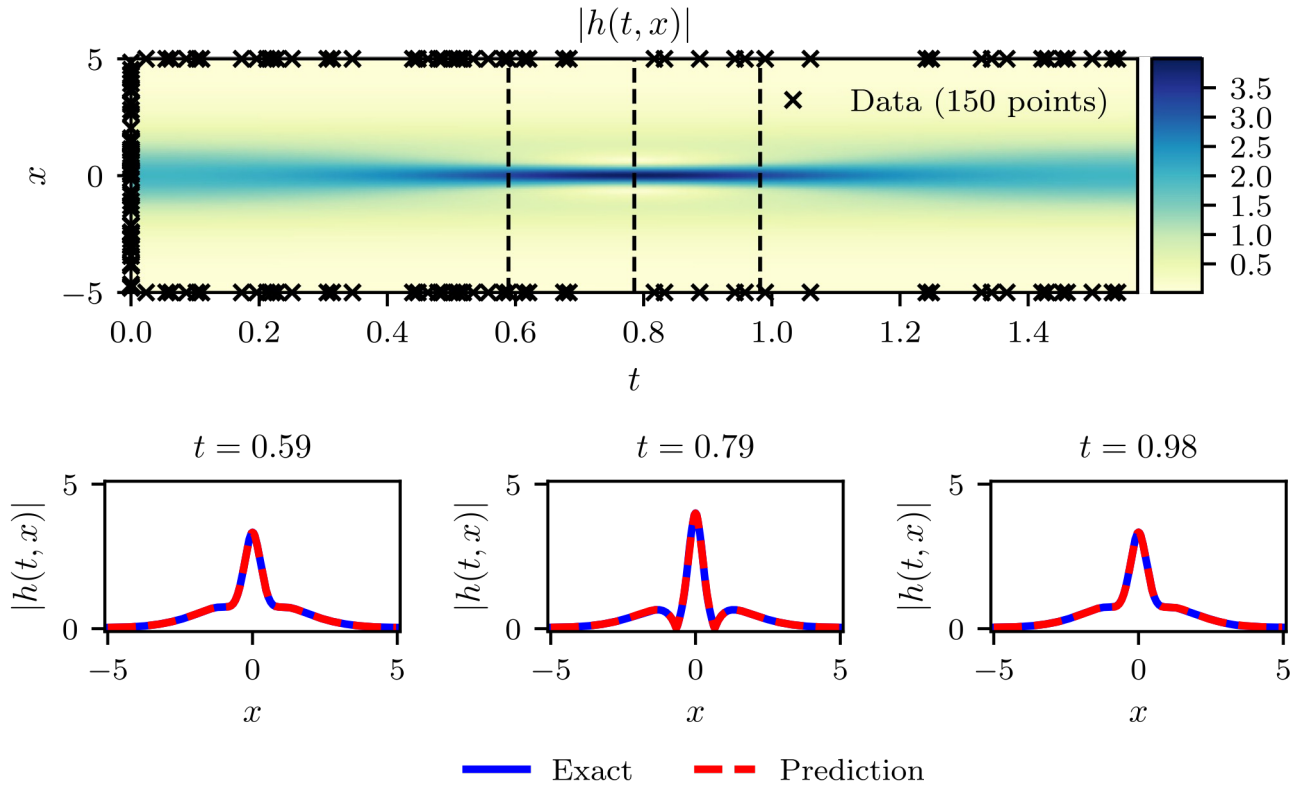
Physics-Informed Neural Networks (PINNs) - Examples

Learn solutions of the **Schrödinger equation** (wave propagation)

Note: **no ground-truth values** of $h(t,x)$ are required to train the NN!

- Only $h(0,x)$ (initial conditions) + periodic boundaries



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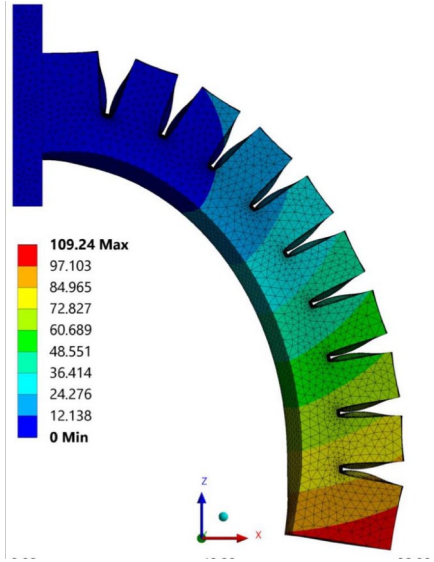
Physics-Informed Neural Networks (PINNs) - Examples



Predict the **deformation** of a pneumatic **soft robot finger**

Continuum mechanics PDE (Navier-Cauchy model):

$$f := (\lambda + \mu)\frac{\partial}{\partial x}(u_x + u_z) + \mu\left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial z^2}\right) + f_x$$

$$g := (\lambda + \mu)\frac{\partial}{\partial z}(u_x + u_z) + \mu\left(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_z}{\partial z^2}\right) + f_z$$

u_x, u_z = deformations along x and z, f_x, f_z = body forces due to gravity

Loss function: $\mathcal{L} = \mathcal{L}_{u_x,u_z} + \mathcal{L}_{f,g}$

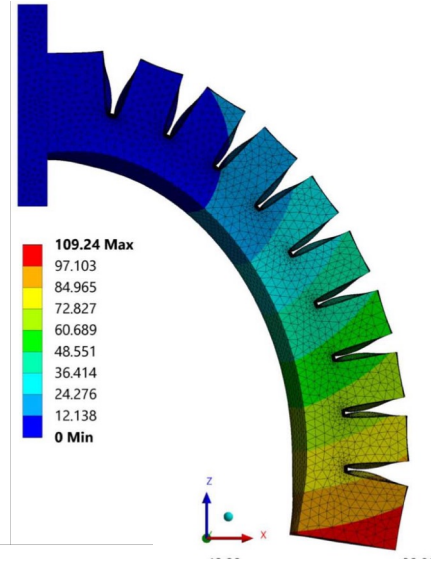
Initial condition: $$\mathcal{L}_{u_x,u_z} = \frac{1}{N}\sum_{i=1}^{N}\left(\left|\hat{u}_x^i - u_x^i\right|^2 + \left|\hat{u}_z^i - u_z^i\right|^2\right)|_{p^i}$$

Navier-Cauchy eq.: $$\mathcal{L}_{f,g} = \frac{1}{N}\sum_{i=1}^{N}\left(\left|f(x^i, z^i)|_{p^i}\right|^2 + \left|g(x^i, z^i)|_{p^i}\right|^2\right)$$

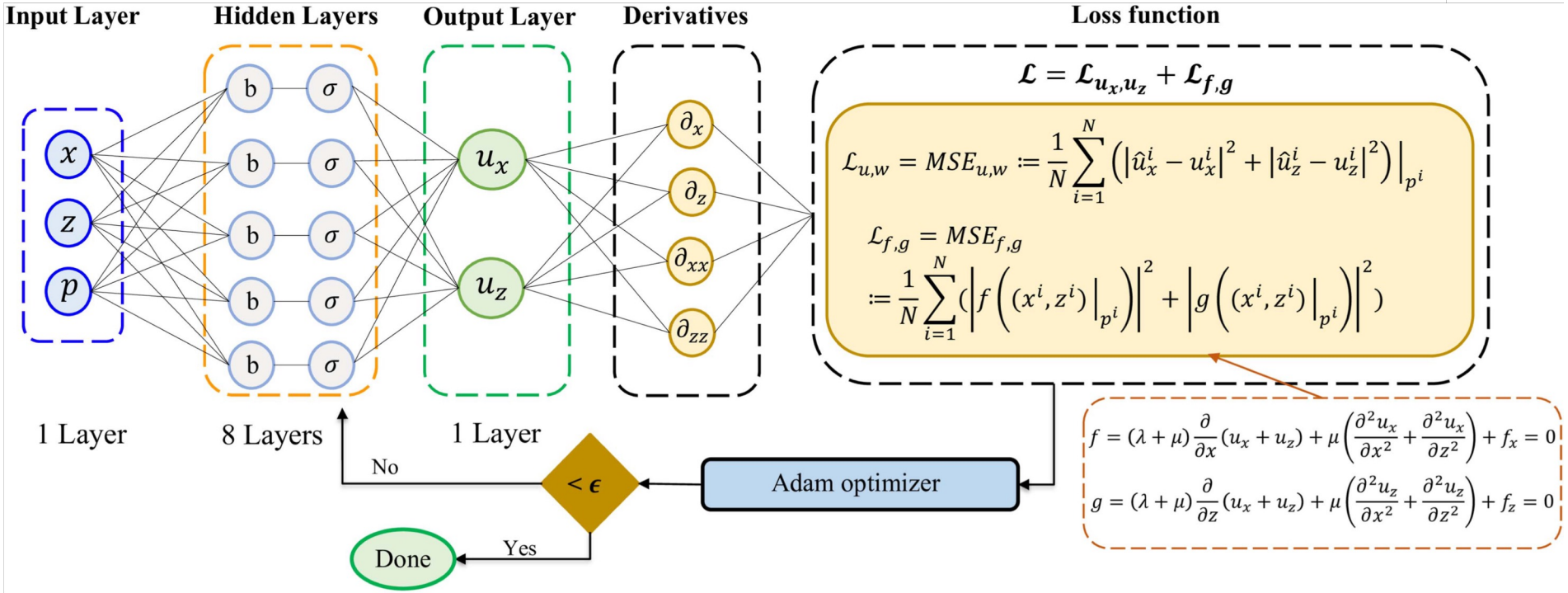
S. Beaber, Z. Liu, Y. Sun, “Physics-Guided Deep Learning Enabled Surrogate Modeling for Pneumatic Soft Robots”, *IEEE RA-L*, 2024

Physics-Informed Neural Networks (PINNs) - Examples

Predict the **deformation** of a pneumatic **soft robot finger**



- **PINN** to learn the deformations u_x, u_z from x, z, applied air pressure p
- Benchmarking against **numerical PDE solution** (FEA with ANSYS)



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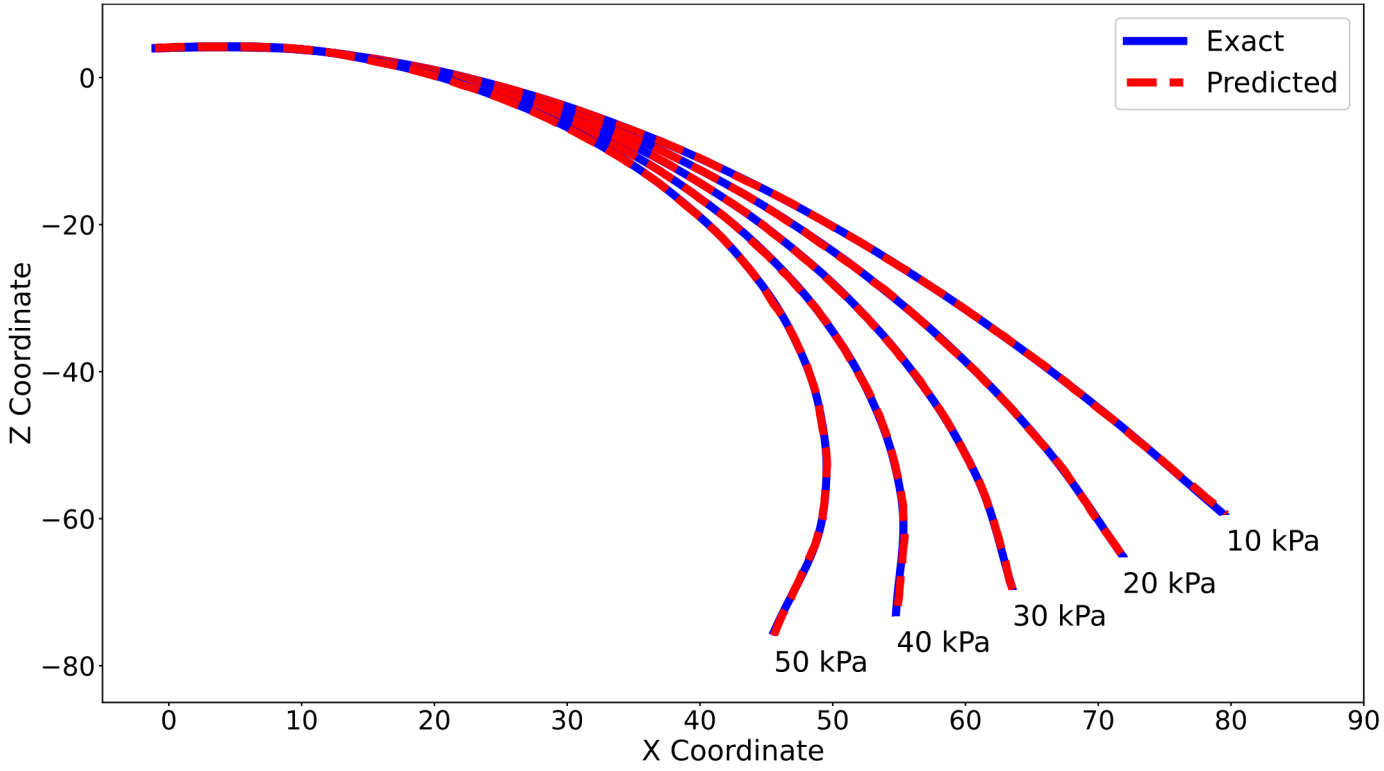
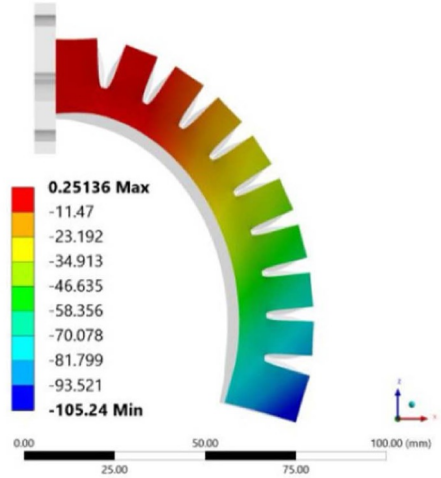
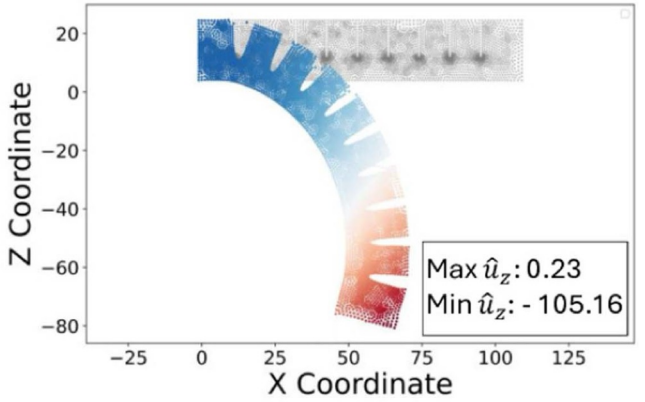
Physics-Informed Neural Networks (PINNs) - Examples

The trained PINN enables **real-time** deformation prediction (way faster than FEA solver)





(a) FEA deformation at 50 kPa



(d) Predicted deformation at 50 kPa

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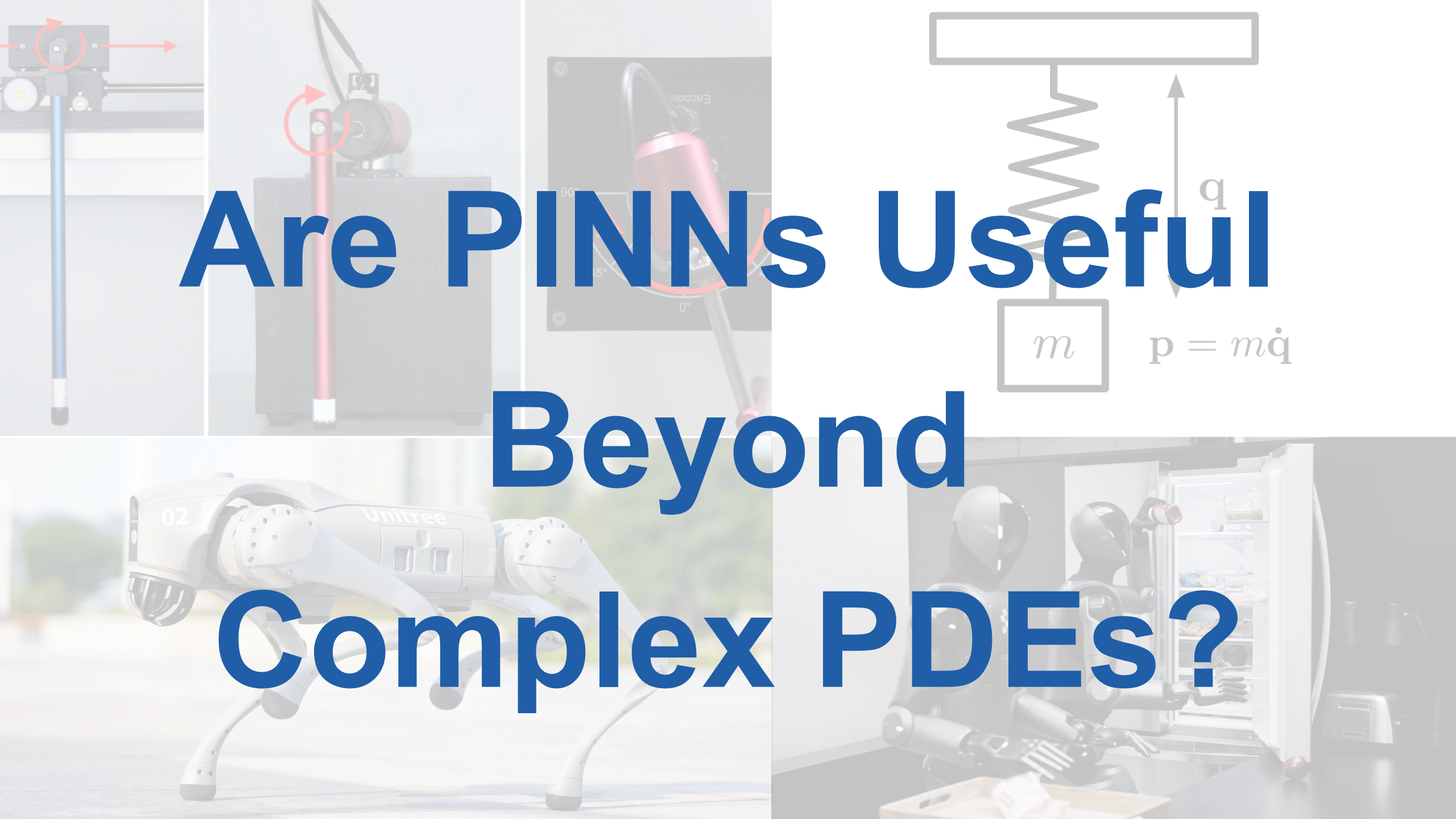

Are PINNs Useful Beyond Complex PDEs?

Physics-Informed Neural Networks (PINNs) - Examples

Learn the **dynamics of a quadrotor**

Quadrotor **dynamics**: Ordinary Differential Equation (**ODE**)

$$\dot{x}(t) = v_x(t),\ \ \dot{y}(t) = v_y(t),\ \ \dot{z}(t) = v_z(t)$$

$$\dot{v}_x(t) = \left(c_{\phi(t)} s_{\theta(t)} c_{\psi(t)} + s_{\phi(t)} s_{\psi(t)}\right) \frac{u_p(t)}{m}$$

$$\dot{v}_y(t) = \left(c_{\phi(t)} s_{\theta(t)} s_{\psi(t)} - s_{\phi(t)} c_{\psi(t)}\right) \frac{u_p(t)}{m}$$

$$\dot{v}_z(t) = -g + c_{\phi(t)} c_{\theta(t)} \frac{u_p(t)}{m}$$

$$\dot{\phi}(t) = \omega_1(t),\ \ \dot{\theta}(t) = \omega_2(t),\ \ \dot{\psi}(t) = \omega_3(t)$$

$$\dot{\omega}_1(t) = \frac{J_2 - J_3}{J_1} \omega_2(t)\omega_3(t) + \frac{J_p}{J_1} \omega_p(t)\omega_2(t) + \frac{1}{J_1} \tau_1(t)$$

$$\dot{\omega}_2(t) = \frac{J_3 - J_1}{J_2} \omega_1(t)\omega_3(t) - \frac{J_p}{J_2} \omega_p(t)\omega_1(t) + \frac{1}{J_2} \tau_2(t)$$

$$\dot{\omega}_3(t) = \frac{J_1 - J_2}{J_3} \omega_1(t)\omega_2(t) + \frac{1}{J_3} \tau_3(t).$$

$$\partial_t \hat{y} + N[\hat{y}; \lambda] = 0$$

$$l := \partial \hat{y} + N[\hat{y}]$$

Learn $\hat{y}(t)$ with a NN

D. Bianchi, N. Epicoco, M. Di Ferdinando, et al., “Physics-Informed Neural Networks for Unmanned Aerial Vehicle System Estimation”, *Drones*, 2024

Physics-Informed Neural Networks (PINNs) - Examples

Learn the **dynamics of a quadrotor**

$$\partial_t \hat{y} + N[\hat{y}; \lambda] = 0 \quad \Rightarrow \quad l := \partial \hat{y} + N[\hat{y}]$$

Loss function: $$MSE = MSE_{\hat{y}} + \gamma MSE_l$$

Data loss:

$$MSE_{\hat{y}} = \frac{1}{N_{\hat{y}}} \sum_{i=1}^{N_{\hat{y}}} \frac{1}{N_t} \sum_{j=1}^{N_t} |\hat{y}_i(t^j) - \hat{y}^j_{i,ref}|^2$$

N_t = n. data samples

$N_{\hat{y}}$ = n. outputs

Supervised learning with collected training data $\hat{y}_{ref}$

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N_t = n. data samples

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Physics loss:

$$MSE_l = \frac{1}{N_{\hat{y}}} \sum_{i=1}^{N_{\hat{y}}} \frac{1}{N_l} \sum_{j=1}^{N_l} |l(\hat{y}_i(t^k))|^2$$

Penalize violations of physics equations

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Loss function: $MSE = MSE_{\hat{y}} + \gamma MSE_l$ γ weighs our **physics confidence**

Data loss:

$$MSE_{\hat{y}} = \frac{1}{N_{\hat{y}}} \sum_{i=1}^{N_{\hat{y}}} \frac{1}{N_t} \sum_{j=1}^{N_t} |\hat{y}_i(t^j) - \hat{y}^j_{i,ref}|^2$$

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Physics loss:

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N_l = n. collocation points t_k

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Physics-Informed Neural Networks (PINNs) - Examples

Learn the **dynamics of a quadrotor**

Results for parameter estimation:

- **Outperforming** an Extended Kalman Filter (EKF)

Parameter	Value	Units	Known for EKF	Known for PINNs
m	0.65	kg	YES	NO
d	0.165	m	YES	NO
J_x	0.03	$\text{kg} \cdot \text{m}^2$	NO	NO
J_y	0.025	$\text{kg} \cdot \text{m}^2$	NO	NO
J_z	0.045	$\text{kg} \cdot \text{m}^2$	NO	NO
b	3.50	N/rad/s	NO	NO
k	0.06	$\text{N} \cdot \text{m/rad/s}$	NO	NO

Table 3. Performance indices for the x model errors expressed in meters.

	MAE	MSE	ISE	IAE	ITAE
EKF	0.0514	0.0039	5.8711	77.17	599.94
PINNs	0.0367	0.0022	3.3427	55.07	432.52

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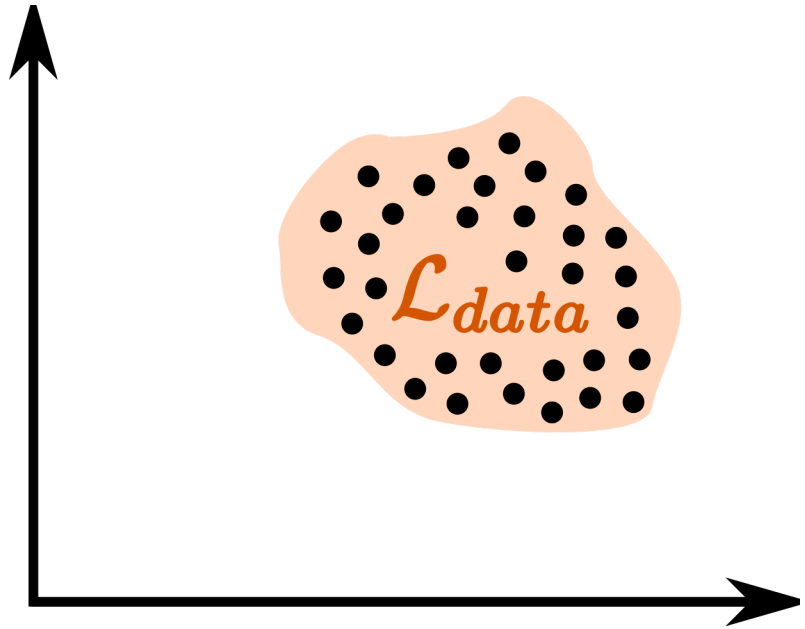
Physics-Informed Neural Networks (PINNs) - Examples

Common approach in **real-world physical systems** & **robotics**

Combine **data + physics *regularization* loss**

$$\mathcal{L} = \mathcal{L}_{data} + \mathcal{L}_{physics}$$



Highly effective when:

- Real **data** is concentrated in **small domain** regions → use $\mathcal{L}_{data}$ there
- We have real **data** measurements + an (imperfect) **physics model**

Physics-Informed Neural Networks (PINNs) - Examples

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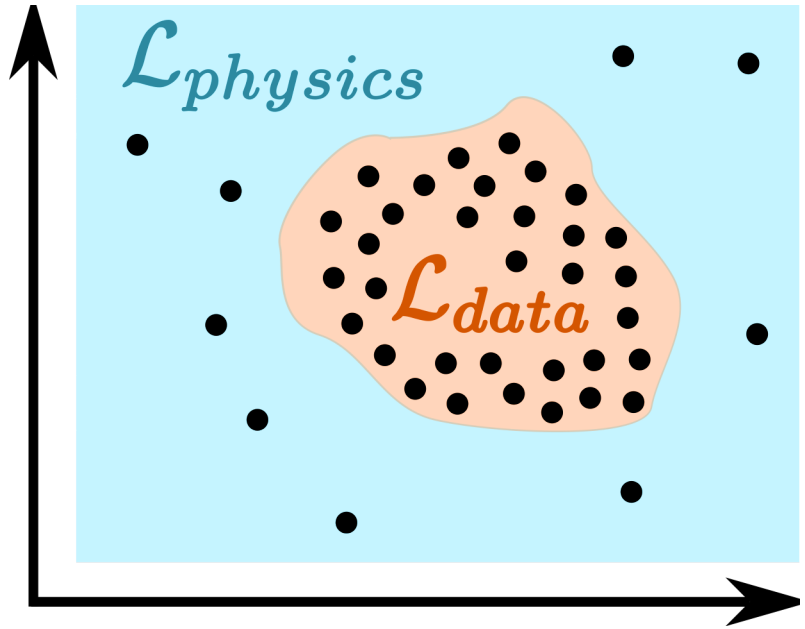


Highly effective when:

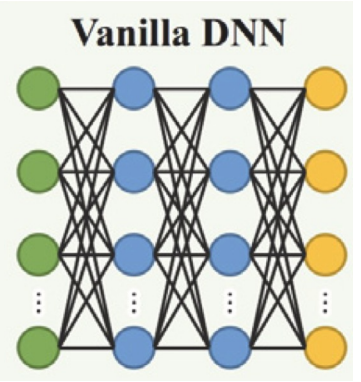
- Real **data** is concentrated in **small domain** regions → use $\mathcal{L}_{data}$ there
- We have real **data** measurements + an (imperfect) **physics model**
- Use $\mathcal{L}_{physics}$ to **generalize** well in data-scarce regions
- Note: $\mathcal{L}_{physics}$ does **not** require ground truth data

Can PINN Loss Function Contain Other Terms?

Physics-Informed Neural Networks (PINNs) - Examples

Learn the **inverse** **dynamics of a quadrotor**

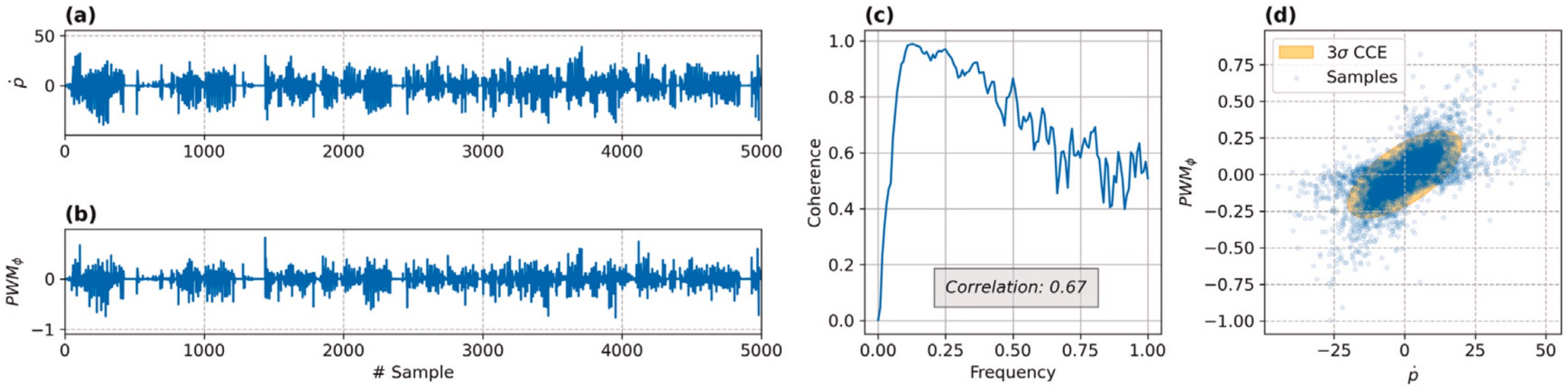
$\hat{\boldsymbol{Y}} = \text{PINN}(\boldsymbol{X}, \boldsymbol{\theta})$, $\boldsymbol{X}$ = quadrotor states, $\hat{\boldsymbol{Y}}$ = control inputs (PWM motor signals)



Loss function idea: Embed **conservation of momentum**

→ Exploit **correlation** of inputs and accelerations:

- **Roll** acceleration $\dot{p}$ highly correlated to PWM motor signal to generate it



W. Gu, S. Primatesta, A. Rizzo, "Physics-informed Neural Network for Quadrotor Dynamical Modeling", *Robotics and Autonomous Systems*, 2024

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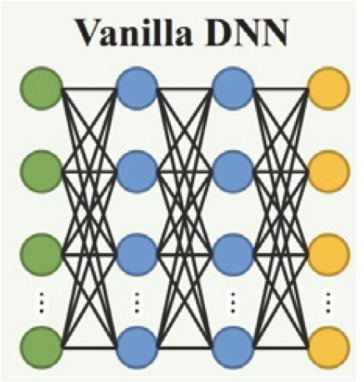
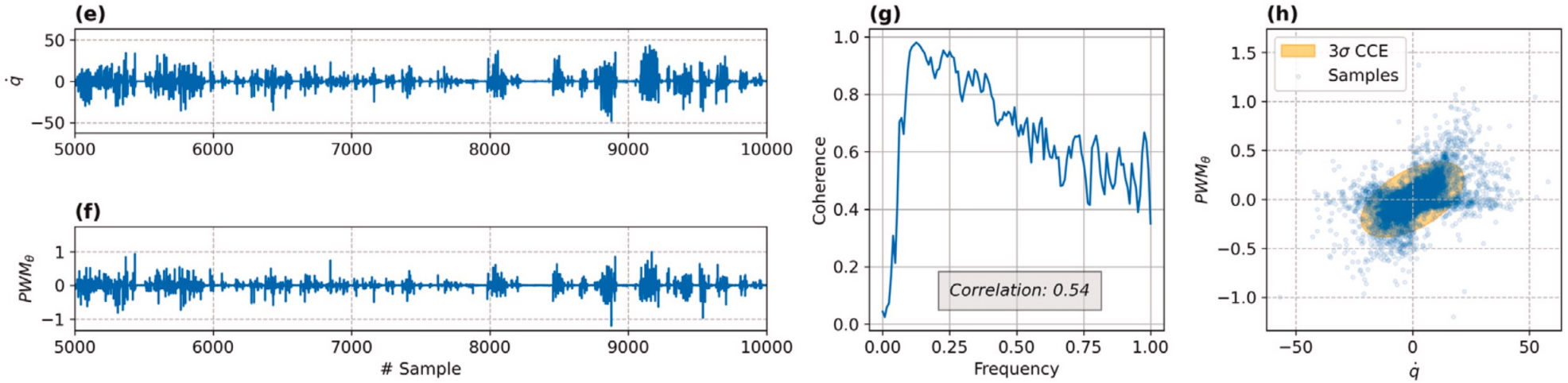


Loss function idea: Embed **conservation of momentum**

→ Exploit **correlation** of inputs and accelerations:

- **Pitch** acceleration $\dot{q}$ highly correlated to PWM motor signal to generate it



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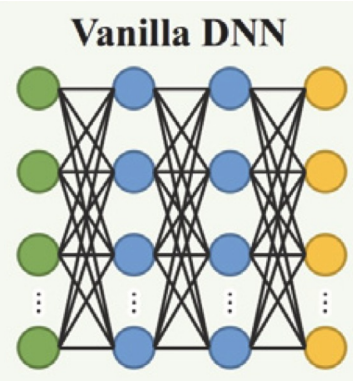
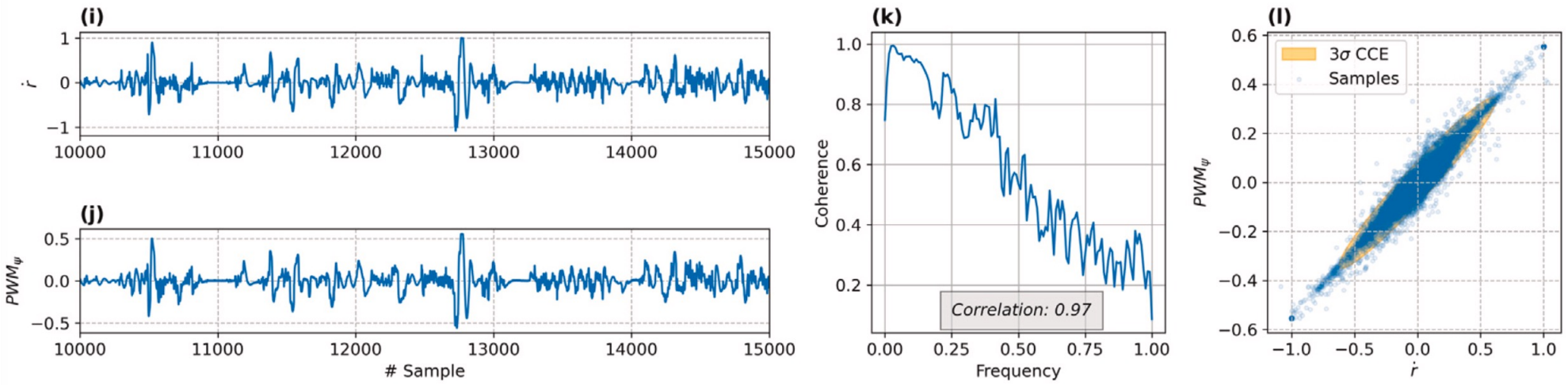


Loss function idea: Embed **conservation of momentum**

→ Exploit **correlation** of inputs and accelerations:

- **Yaw** acceleration $\dot{r}$ highly correlated to PWM motor signal to generate it



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Physics-Informed Neural Networks (PINNs) - Examples

Learn the **inverse dynamics of a quadrotor**

Loss function idea: Embed **conservation of momentum**

→ **Local Monotonicity (LM)** loss terms:

- Accelerations and PWM signals should *exhibit the same pattern*

$$\mathcal{L} = \mathcal{L}_{\text{MSE}} + \sum_i \lambda^i_{\text{LM}} \mathcal{L}^i_{\text{LM}}, \quad i = \{\phi, \theta, \psi\}$$

$\sum_i \lambda^i_{\text{LM}} \mathcal{L}^i_{\text{LM}}$ = local monotonicity loss for the roll, pitch, yaw rotations (**soft constraints**)

$\mathcal{L}_{\text{MSE}}$ = standard data-driven loss → minimize deviations from ground-truth observations

W. Gu, S. Primatesta, A. Rizzo, "Physics-informed Neural Network for Quadrotor Dynamical Modeling", *Robotics and Autonomous Systems*, 2024

Physics-Informed Neural Networks (PINNs) - Examples

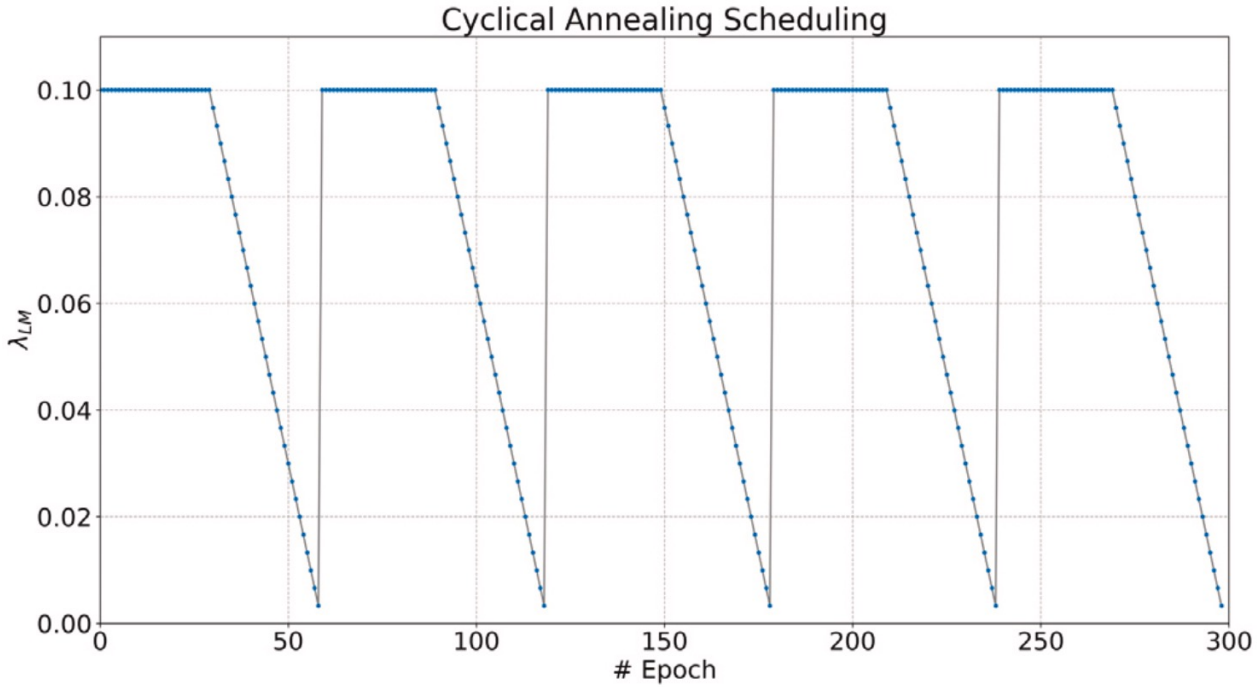
Learn the **inverse dynamics of a quadrotor**

Issue: strong **aerodynamic effects** can **contradict** the local **monotonicity loss**

→ Accelerations and motor commands may no longer be highly correlated!

→ **Cyclical annealing scheduler** for the LM terms to let the NN **learn real aerodyn.** effects

$$\mathcal{L} = \mathcal{L}_{\text{MSE}} + \sum_i \lambda_{\text{LM}}^i \mathcal{L}_{\text{LM}}^i,$$



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Questions & Discussion

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