

# Physics-Grounded Machine Learning

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June 8, 2023

MITSUBISHI ELECTRIC RESEARCH LABORATORIES (MERL)

Cambridge, Massachusetts, USA

<http://www.merl.com>

# Mitsubishi Electric Corporation

- Main businesses and product examples:



**Air Conditioning Systems**



**Automotive Equipment**



**Building Systems**



**Energy Systems**



**Factory Automation Systems**



**Home Products**



**Information & Comm. Systems**



**Public Systems**



**Semiconductors & Devices**



**Space Systems**



**Transportation Systems**



**Visual Information Systems**

- \$40B revenues with strong growth plans
- NOT Mitsubishi Motors, Mitsubishi Heavy Industries, ...

# MERL Profile & Research Areas

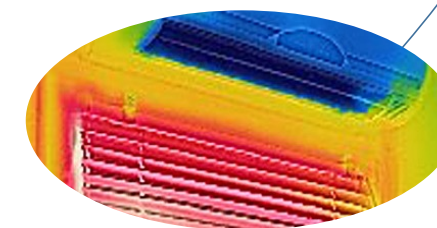
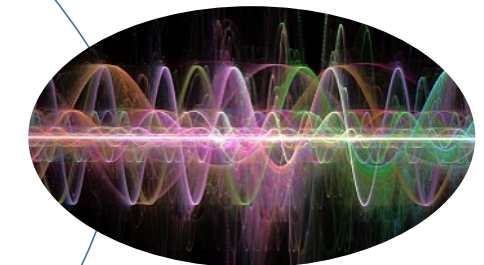
- MERL was founded in 1991 in Cambridge, Mass
- Very academically-oriented and open industrial research labs, publishing almost everything
  - 60 PhD researchers, working in multiple disciplines
  - 150+ papers per year
  - Many university collaborations
- Engaged in mid/long-term research on topics that we expect to be beneficial to our parent company
- Strong summer internship program
  - 80+ interns throughout the year
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**Artificial Intelligence  
Machine Learning  
Computer Vision  
Speech & Audio**



**Control  
Optimization  
Robotics  
Data Analytics**

**Signal Processing  
Computational Sensing  
Communications  
Electronic Devices**



**Multi-Physical Modeling  
Applied Physics  
Dynamical Systems  
Electric Systems**

## Mitsubishi Electric AI Ethics Policy

<https://www.mitsubishielectric.com/en/sustainability/social/humanrights/aipolicy>

Published 12/15/2021

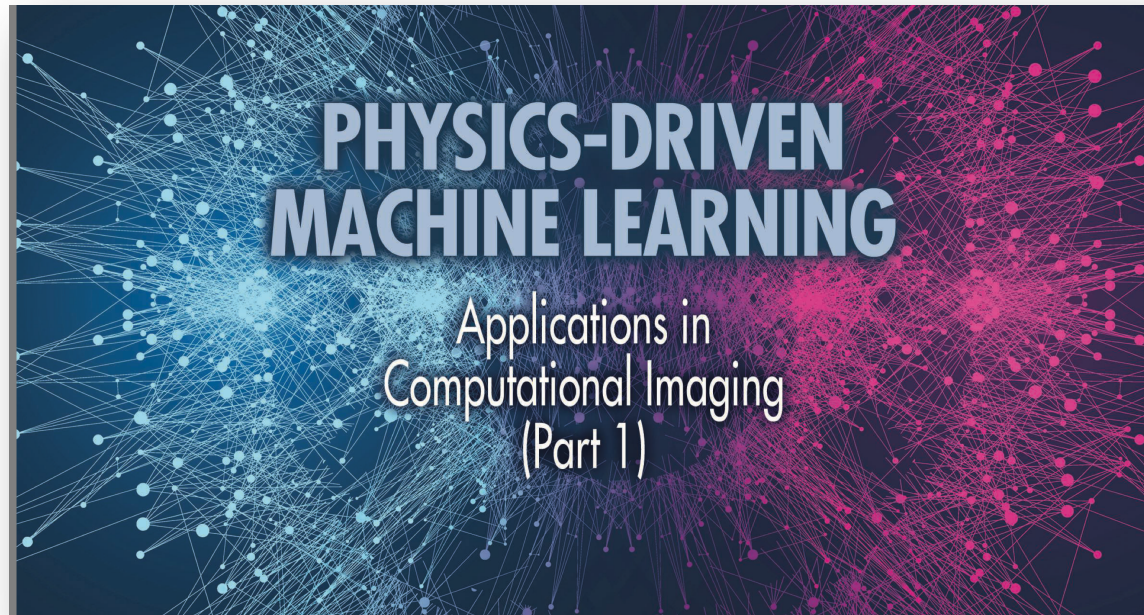
- 1) Realization of a human-centered AI society
- 2) Fair and non-discriminatory utilization
- 3) Ensuring safety and security
- 4) Consideration for privacy
- 5) Transparency and accountability
- 6) Development of AI and human resources
- 7) Compliance with laws and regulations



- Principled design and use of machine learning has become centerstage
- Scientific communities looking hard at the problems around explainable, reliable & sustainable ML [see J-STSP special issue]
- At least for real-world engineering systems, being able to leverage what we know about the physics of these systems could provide a reasonable path forward

# Physics-(Inspired/Informed/Driven/Guided/Grounded) ML

- Terms might carry different meaning for different people and communities, but they are fairly interchangeable (at least to me)




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## Physics-informed machine learning

[George Em Karniadakis](#) , [Ioannis G. Kevrekidis](#), [Lu Lu](#), [Paris Perdikaris](#), [Sifan Wang](#) & [Liu Yang](#)

[Nature Reviews Physics](#) **3**, 422–440 (2021) | [Cite this article](#)

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- All methods and approaches aiming to enforce physical principles and constraints, while leveraging the power of data-driven machine learning techniques

# The Physics-Data Spectrum and PIML

## PHYSICS-AGNOSTIC MACHINE LEARNING

- No physics-oriented model, based entirely on data
- Data-driven design, need (often, a lot of) data
- Fragile certificates – at mercy of data generating process

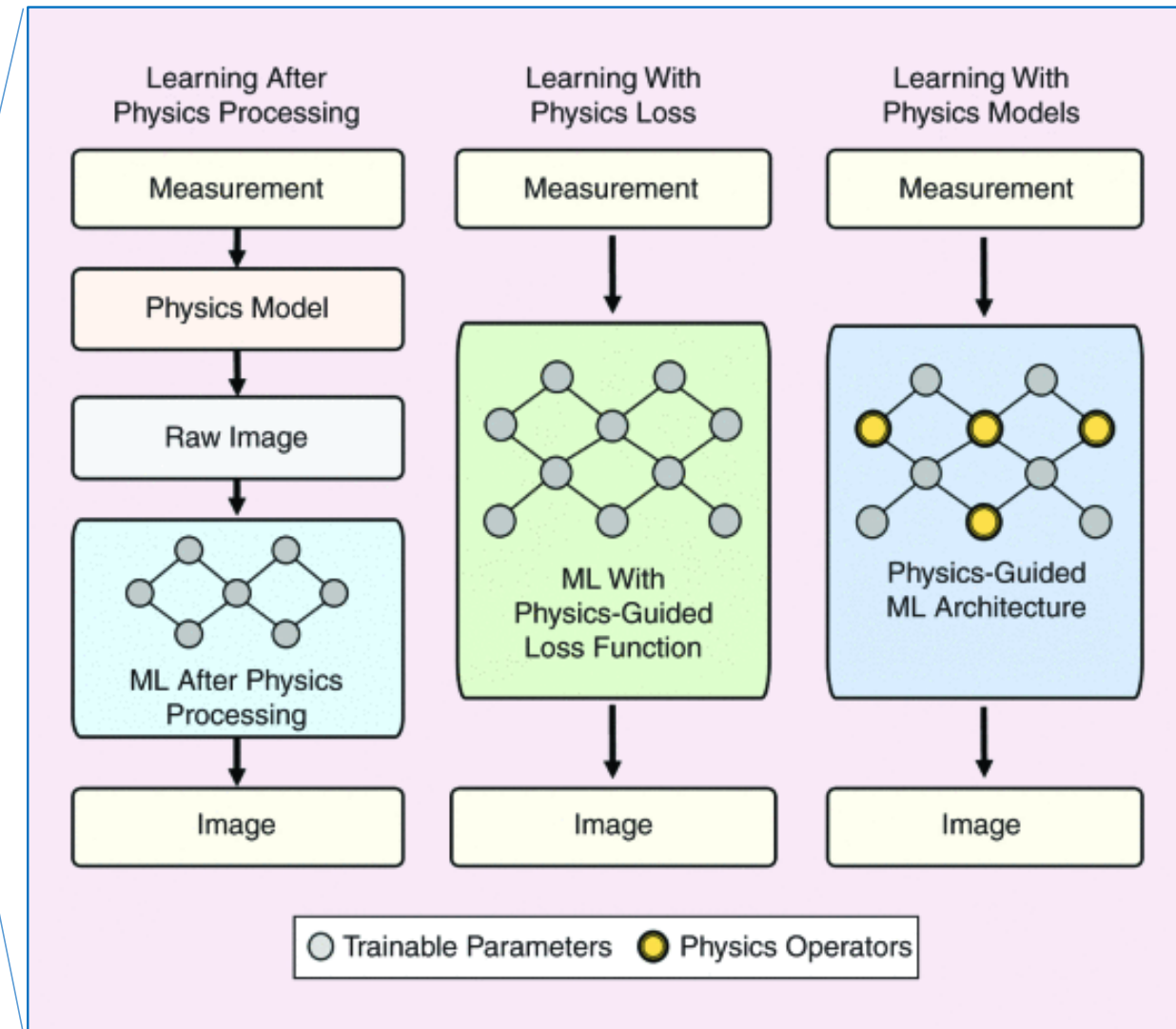
## PHYSICS-INFORMED MACHINE LEARNING (PIML)

- Embed physics-based knowledge into machine learning methods
- More performance-optimal design possible with data injection
- Performance certificates more robust

## PHYSICS-BASED DESIGN

- Based entirely on physical knowledge
- Model-environment mismatch can lead to suboptimal design
- Can certify performance

## Exemplar PIML Mechanisms

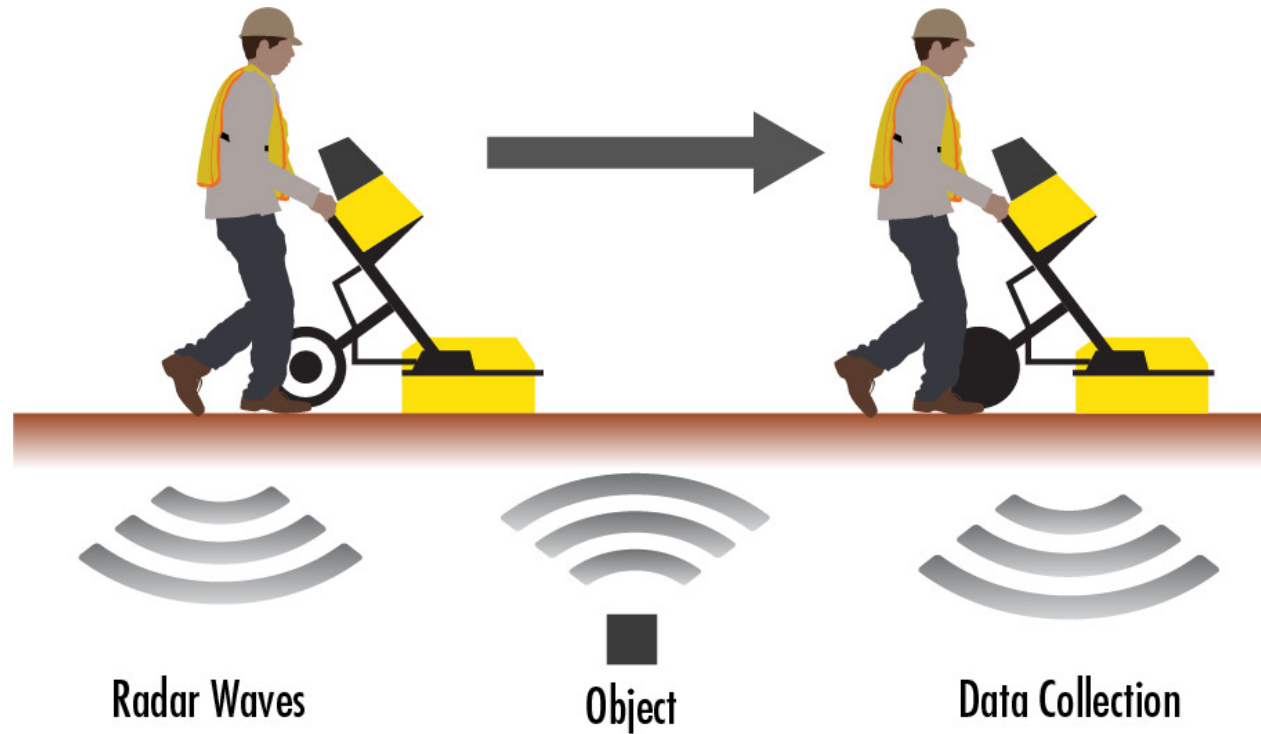


[Guo, et al. SPM 2023]

# Outline & Goals for Rest of Talk

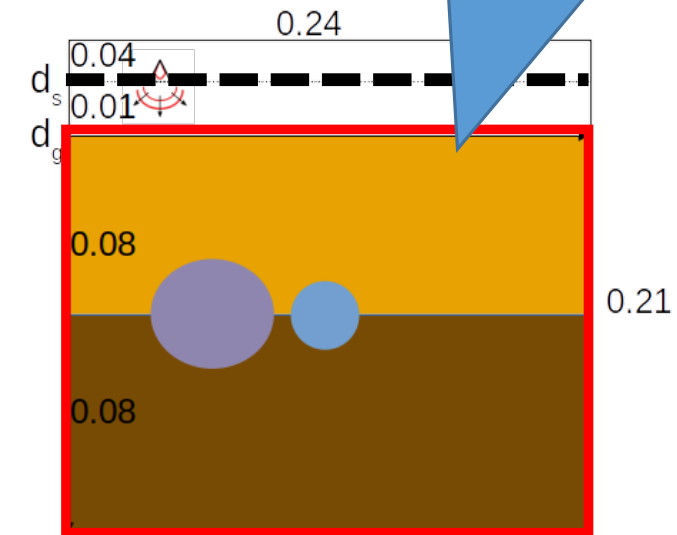
- Walkthrough some practical industrial problems where physics-grounded ML can be used
  - Underground imaging of infrastructure
  - Imaging of hazardous gases
  - Airflow estimation for optimization & control
  - System ID & driving adaptation for autonomous vehicles
- Highlight benefits of PGML, as well as key differences in problem setup and approaches
- Future outlook and perspectives

# Underground Imaging



## Problem Formulation

Reconstruct underground structure & permittivity distribution from sparse surface measurement



$$f = \operatorname{argmin}_f \sum_{\omega} \frac{1}{2} \|y_{\omega} - HZ(\omega, f)\|_2^2 + R(f)$$

Ill-posed due to sparse measurements  
High computational cost  
Hard to formulate

$f$ : underground structure/permittivity distribution

$\omega$ : frequency

$y_{\omega}$ : ground truth measurements

$H$ : sensor selection mask – selects the sensor measurements

$Z$ : forward model - takes frequency,  $\omega$ , and structure  $f$  as input, and predicts the wavefield



# Conventional Approaches

## 1) Purely analytical

Build relationship between “measurement” and “velocity field” via Lippmann-Schwinger equation and solve via optimization

### Challenges:

- Linear model is easy to formulate but less accurate
- Exact model is hard to formulate for complicated backgrounds
- Problem is Ill-posed due to sparse measurements
- Slow computation for large domains

where

$$\mathbf{f}^* = \arg \min_{\mathbf{f} \in \mathbb{R}^N} \{ \mathcal{F}(\mathbf{f}) := \mathcal{D}(\mathbf{f}) + \mathcal{R}(\mathbf{f}) \},$$

$$\mathcal{D}(\mathbf{f}) = \frac{1}{2} \|\mathbf{y} - \mathcal{Z}(\mathbf{f})\|_2^2,$$

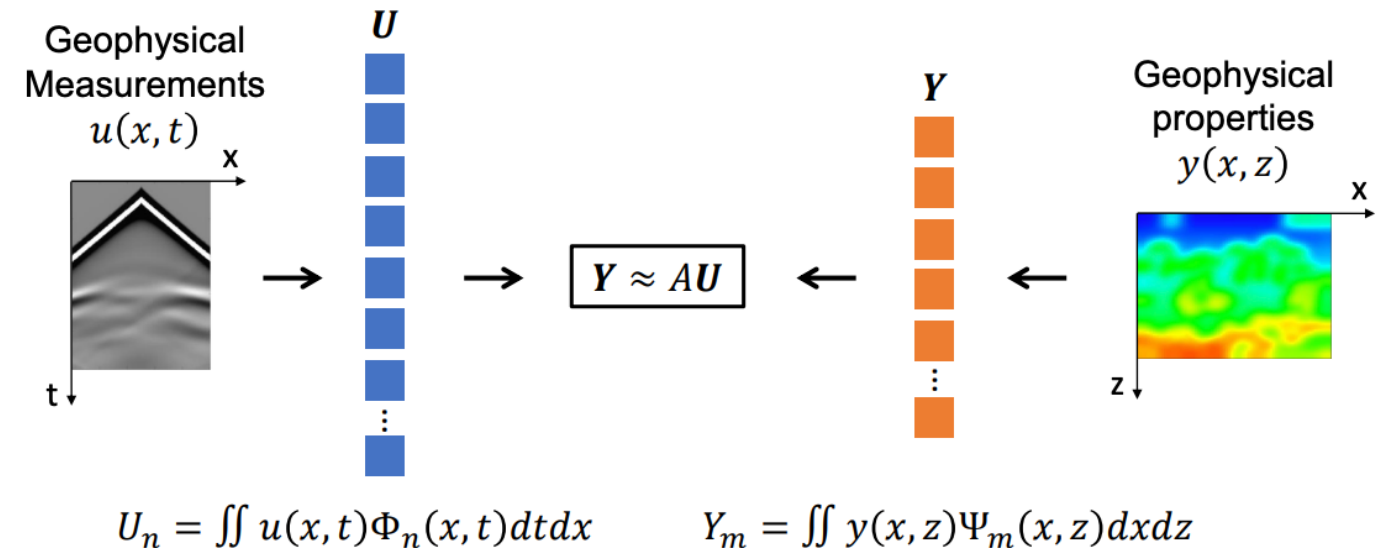
$$\mathcal{R}(\mathbf{f}) = \tau \sum_{n=1}^N \sqrt{\sum_{d=1}^2 |[\mathbf{D}_d \mathbf{f}]_n|^2} + \chi_C(\mathbf{f}).$$

## 2) Purely data-driven

Learn direct mapping via machine learning

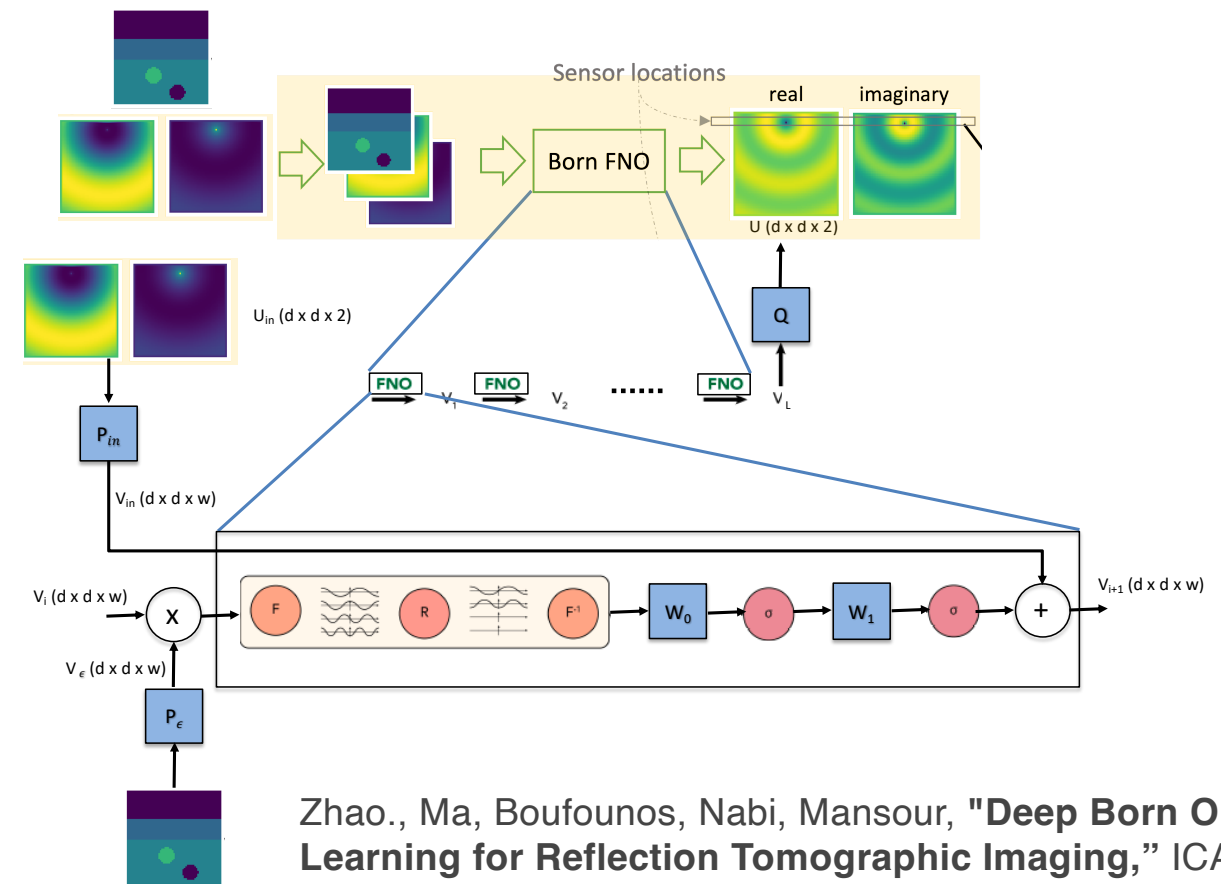
### Challenges:

- Require more data for reasonable generalization
- Only works for the set of sensor locations used during training



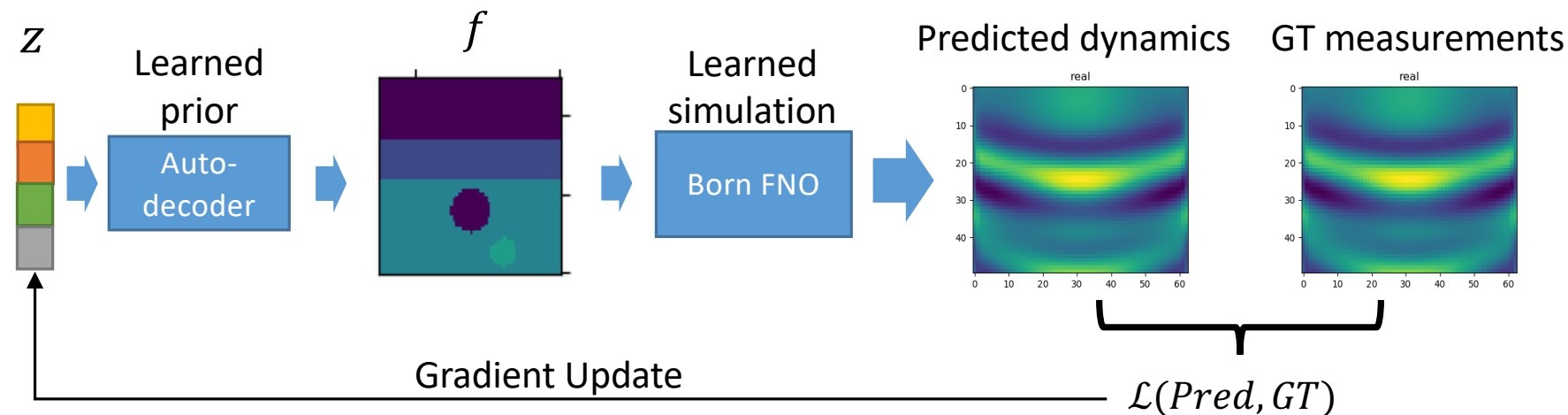
# Physics-Ground ML Model

- Learn the relationship between structure and measurements (forward model  $Z$ )
  - Faster and more general than classical approach (via Lippmann-Schwinger equation)
  - Iterative Born approximates the LS inversion
  - Designed ML architecture that mimics iterative Born for more accurate reconstruction

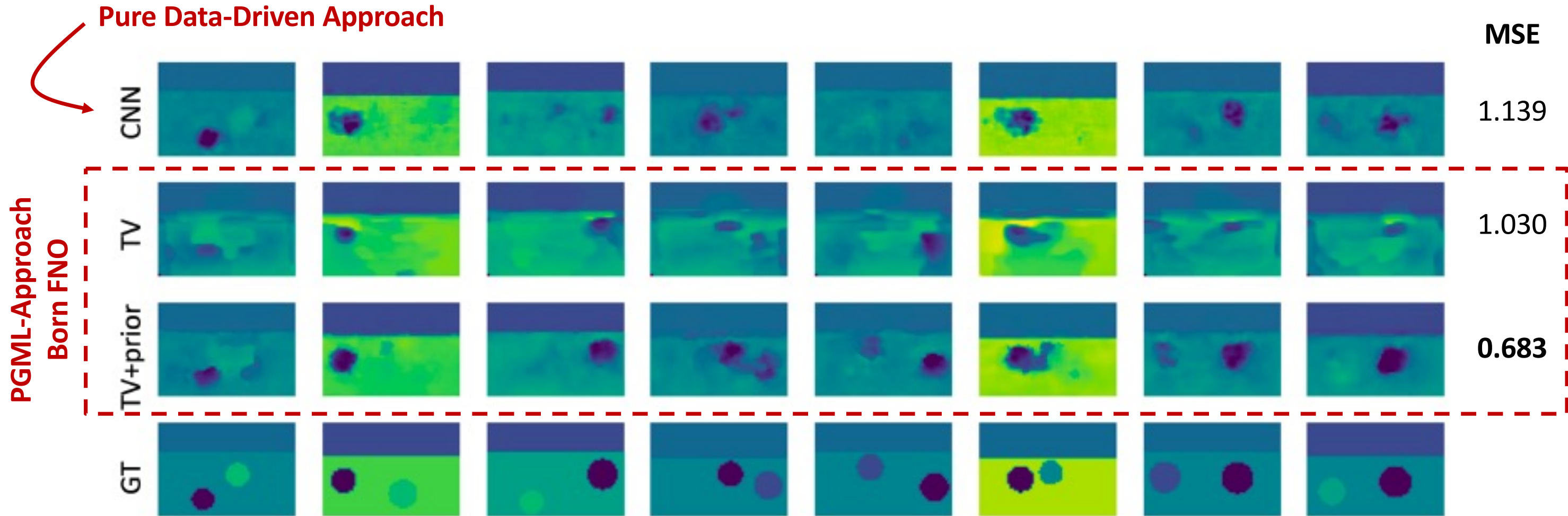


Zhao., Ma, Boufounos, Nabi, Mansour, "Deep Born Operator Learning for Reflection Tomographic Imaging," ICASSP'23.

- Leverage auto-encoder prior to learn the distribution of underground images



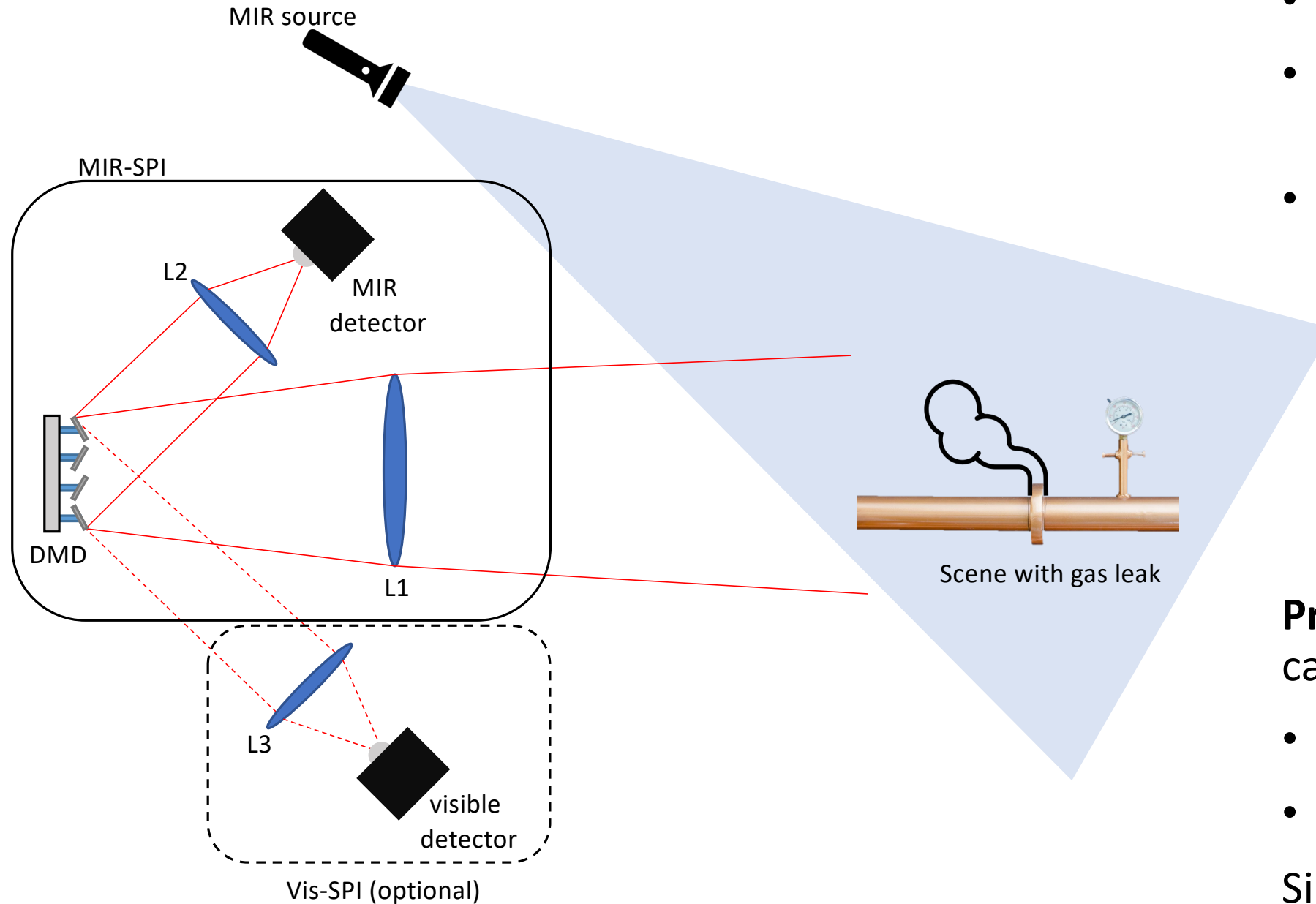
# Experimental Results



## RECAP

- Learn both propagation dynamics and underground image model
- Use PGML-approach to model the propagation

# Single-Pixel Imaging of Hazardous Gases



## Objective & Issues

- Target low-cost imaging of hazardous gases
- Certain hazardous gases are only visible in medium infrared (MIR)
- CMOS/CCD arrays only go up to near-IR, so MIR arrays are very expensive

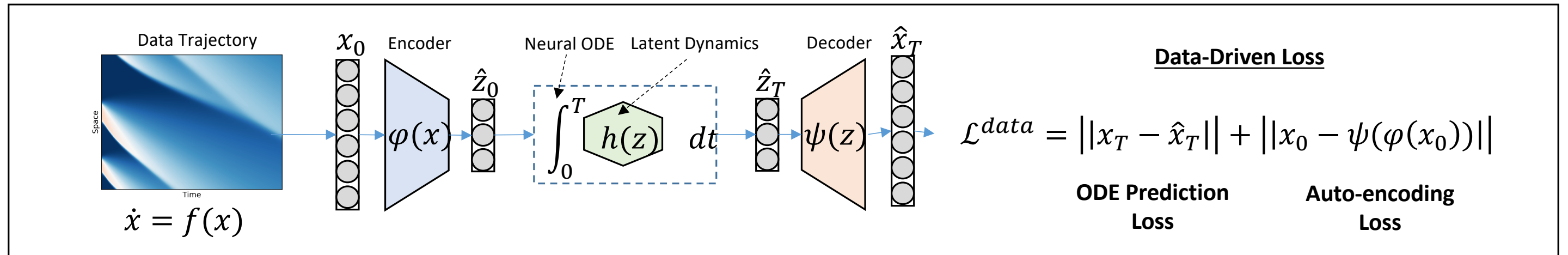
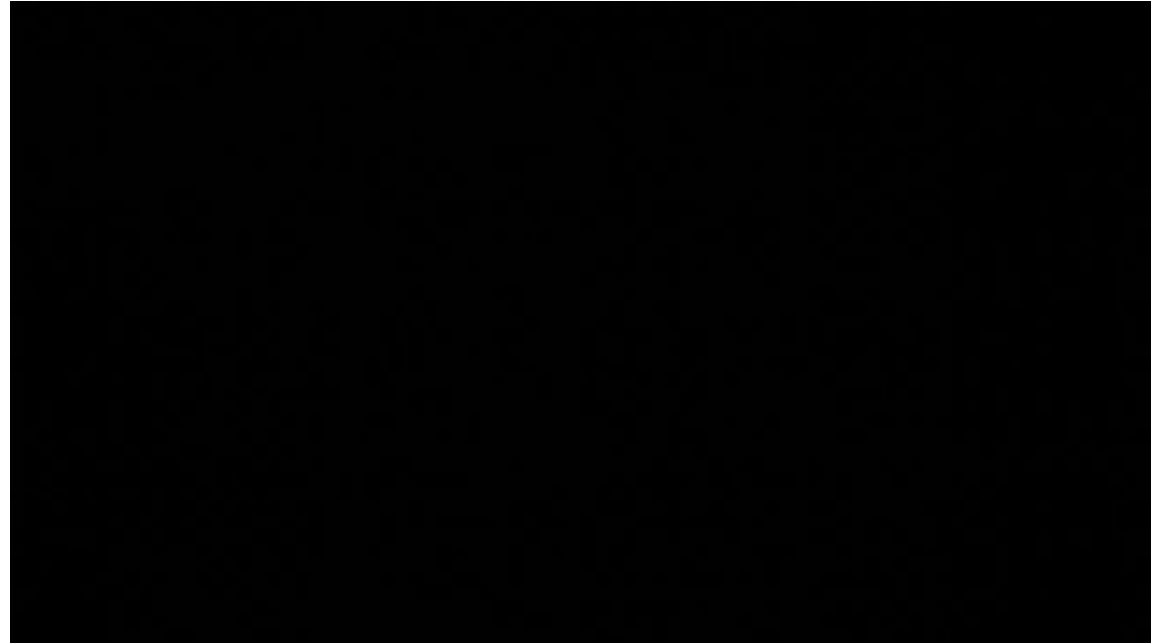
**Proposed Design:** Consider single-pixel camera architecture consisting of

- Digital micro-mirror device (DMD)
- Single-pixel MIR detector

Since fast DMD is expensive, target acquisition that works with few snapshots

# Learning the Dynamics of Gas for Image Reconstruction

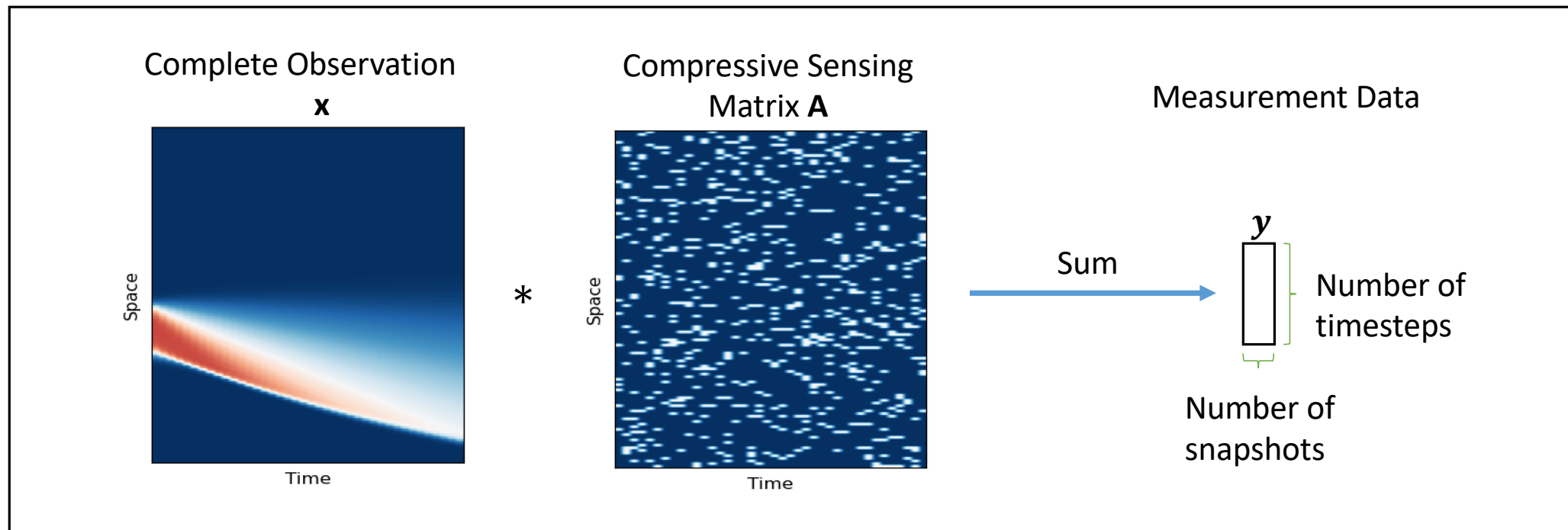
- Gases can change dynamically over time.
- We model the evolution of the gas over time using a dynamical system model that constrains the reconstruction.
- A dynamical model of a gas can be written as:  
 $\dot{x} = f(x)$  where  $f(x)$  defines the system model  
 e.g., Navier-Stokes equation
- Since  $f(x)$  is difficult to solve, we learn the dynamics from examples.



# Measurement Model & Data

$$y = Ax$$

- $x$  is the observation data (sequence of images of the gas cloud as it changes over time)
- Every snapshot that is captured by the DMD corresponds to a single row in a measurement matrix  $A$
- $y$  is the measurement data (sequence of snapshots acquired within some duration of time)



**NOTE:** In contrast to the previous underground imaging setup

- Measurement model in this problem is linear and known (DMD pattern)
- PGML only used to learn the observed signal dynamics (gas flow)

# Reconstruction Approach

Given the data and learned dynamics, we determine a solution that explains the data and satisfies the ODE constraints

Reconstruction  
Loss

Compressive  
Sensing Loss

Loss for Prediction in  
Latent space

$$\mathcal{L}^{recon.}(z) = \underbrace{\|y - A\psi(z)\|}_{\text{Compressive Sensing Loss}} + \underbrace{\left\| z - \left( z_0 + \int_0^T h(z) dz \right) \right\|}_{\text{Loss for Prediction in Latent space}}$$

Latent-space  
representation  
of the trajectory

*What the data tells us  
the trajectory should be*

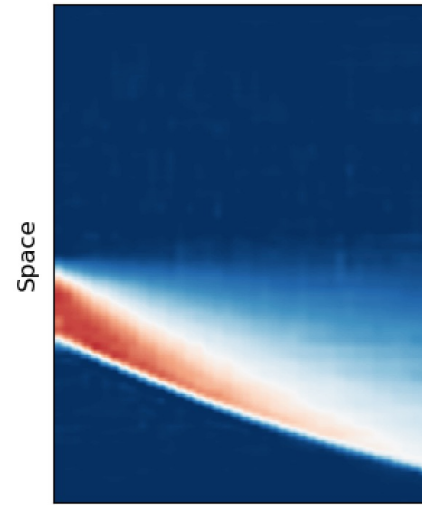
*What the model thinks the  
trajectory should be*

# Experimental Results

- Evaluate on simulated gas dynamics characterized by Burger's equation.
- Train a Neural ODE operator to learn dynamics with variety of initial conditions propagated through the same PDE.
- Test on a new set of dynamics observed using a single pixel imaging setup applied to a one-line DMD sensor.

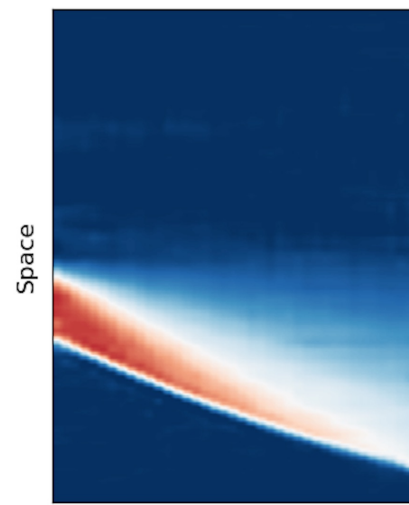
Results show that utilization of physical model can accurately reconstruct the images of the fluid with 1/16th the number of measurements as conventional single pixel imaging algorithms.

Our method  
[32 samples/frame]



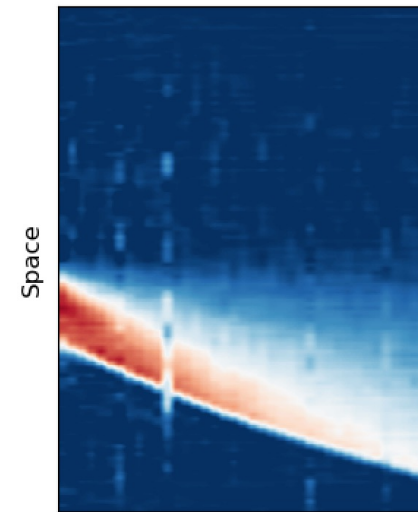
Time

Our method  
[2 samples/frame]



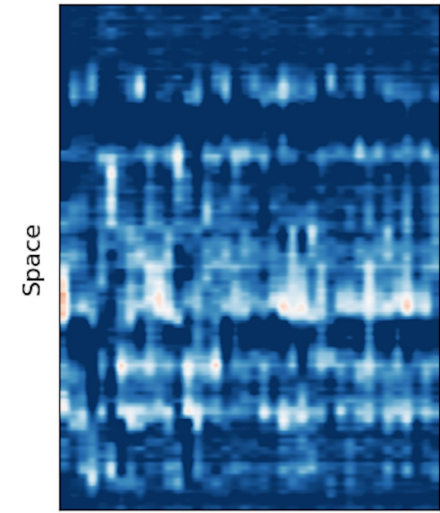
Time

AE w/out Dynamics  
[32 samples/frame]

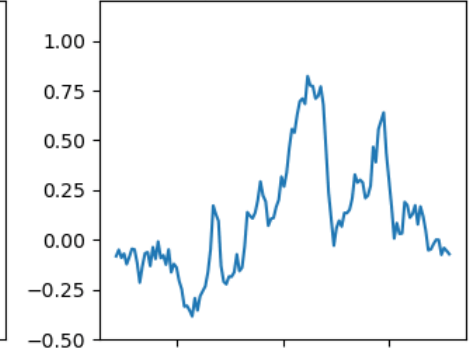
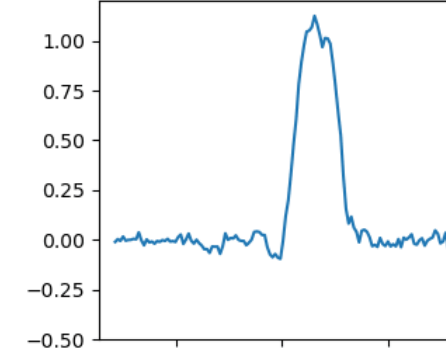
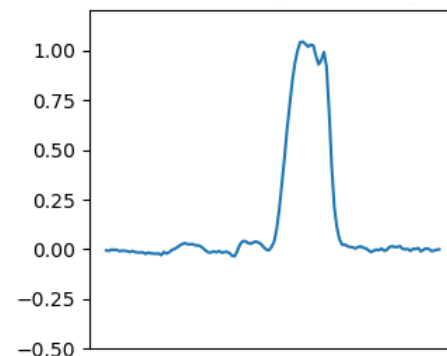
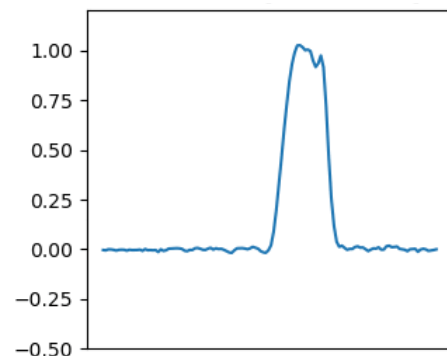
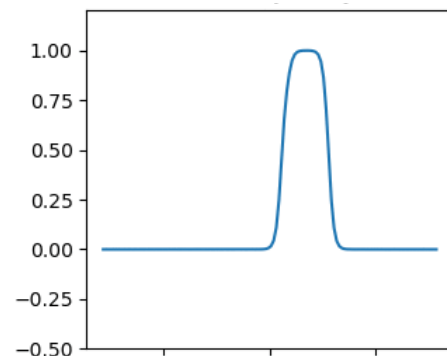


Time

AE w/out Dynamics  
[2 samples/frame]



Time





# Airflow Estimation for Optimization & Control

- Closed-loop feedback control of dynamics systems governed by PDEs, such as airflow in a room, requires a **real-time estimate of the current state from sparse measurements**
- Standard estimation/filtering techniques don't apply
  - High-dimensionality of the system
  - Nonlinearity of the dynamics
  - Dependency on unknown physical parameters

- **Governing parametric PDE**, in discretized form:

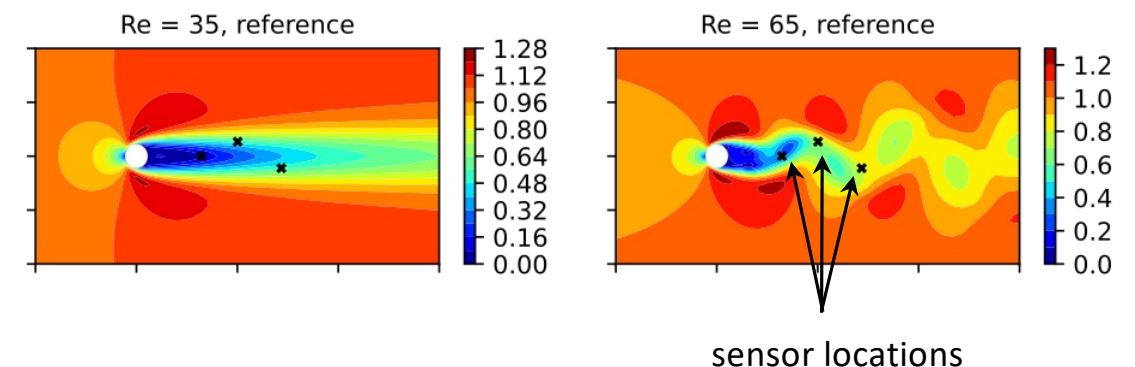
$$\begin{aligned} \mathbf{z}_{k+1} &= \mathbf{f}(\mathbf{z}_k; \boldsymbol{\mu}) && \text{state } \mathbf{z}_k \in \mathbb{R}^n, \text{ parameter } \boldsymbol{\mu} \in \mathbb{R}^l \\ \mathbf{y}_k &= \mathbf{C}\mathbf{z}_k && \text{measurement } \mathbf{y}_k \in \mathbb{R}^p \end{aligned}$$

- **State estimation problem:**

Given time series of sparse measurements  $\{\mathbf{y}_0, \dots, \mathbf{y}_k\}$ , estimate the state  $\mathbf{z}_k$  without direct knowledge of  $\boldsymbol{\mu}$

- **Examples with Navier-Stokes as the PDE:**

- Airflow in a room: parameter  $\boldsymbol{\mu}$  is outside temperature, number of people, ...
- Flow past a cylinder: parameter  $\boldsymbol{\mu}$  the Reynolds number  $Re$



# Reinforcement Learning (RL) for Airflow Estimation

**Training dataset:** Solution trajectories  $\{\mathbf{z}_0, \dots, \mathbf{z}_k\}$  for  $\mu = \mu^{(1)}, \dots, \mu^{(q)}$

**Step 1.** Construct reduced-order model (ROM)

**Step 2.** Construct reduced-order state estimator (ROE)

## Parametric discretized PDE

$$\begin{aligned} \mathbf{z}_{k+1} &= \mathbf{f}(\mathbf{z}_k; \boldsymbol{\mu}) & \text{state } \mathbf{z}_k &\in \mathbb{R}^n \\ \mathbf{y}_k &= \mathbf{C}\mathbf{z}_k & \text{measurement } \mathbf{y}_k &\in \mathbb{R}^p \end{aligned}$$

↓  
reduced state  $\mathbf{x}_k = \mathbf{U}^T \mathbf{z}_k \in \mathbb{R}^r$   
 $r \ll n$ ,  $\mathbf{U}$  are  $r$  leading PCA modes

## 'Averaged' ROM over $\mu$

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{A}_r \mathbf{x}_k & \text{reduced state } \mathbf{x}_k &\in \mathbb{R}^r \\ \mathbf{y}_k &= \mathbf{C}_r \mathbf{x}_k & \text{measurement } \mathbf{y}_k &\in \mathbb{R}^p \end{aligned}$$

$\mathbf{A}_r$  approximates the mean dynamics over all training trajectories  $\mu = \mu^{(1)}, \dots, \mu^{(q)}$

## Kalman filter baseline (KF-ROE):

linear; only model-based

$$\hat{\mathbf{x}}_k = \mathbf{A}_r \hat{\mathbf{x}}_{k-1} + \mathbf{K}_k (\mathbf{y}_k - \mathbf{C}_r \mathbf{A}_r \hat{\mathbf{x}}_{k-1})$$

Performs poorly when  $\mathbf{A}_r$  is not a good model (due to changing  $\mu$ , etc)

## Reinforcement learning-trained estimator (RL-ROE):

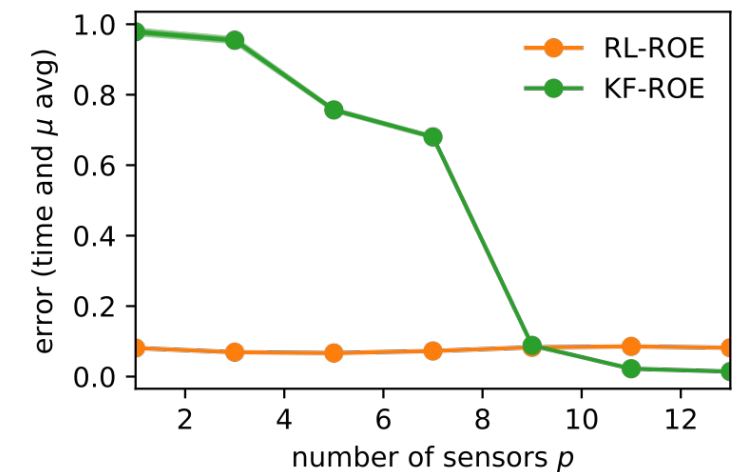
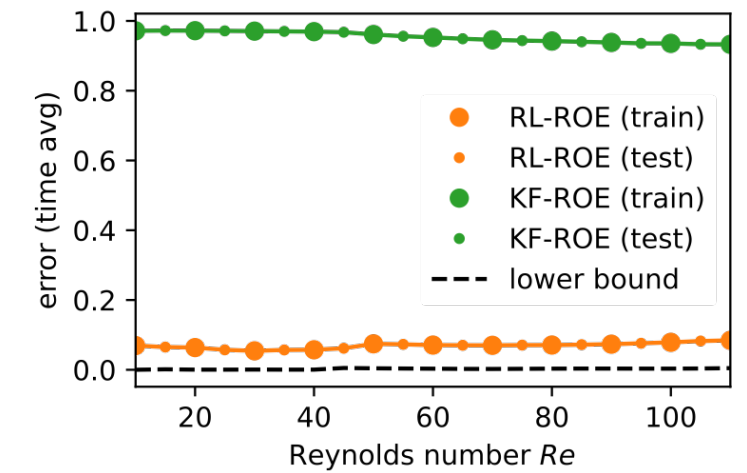
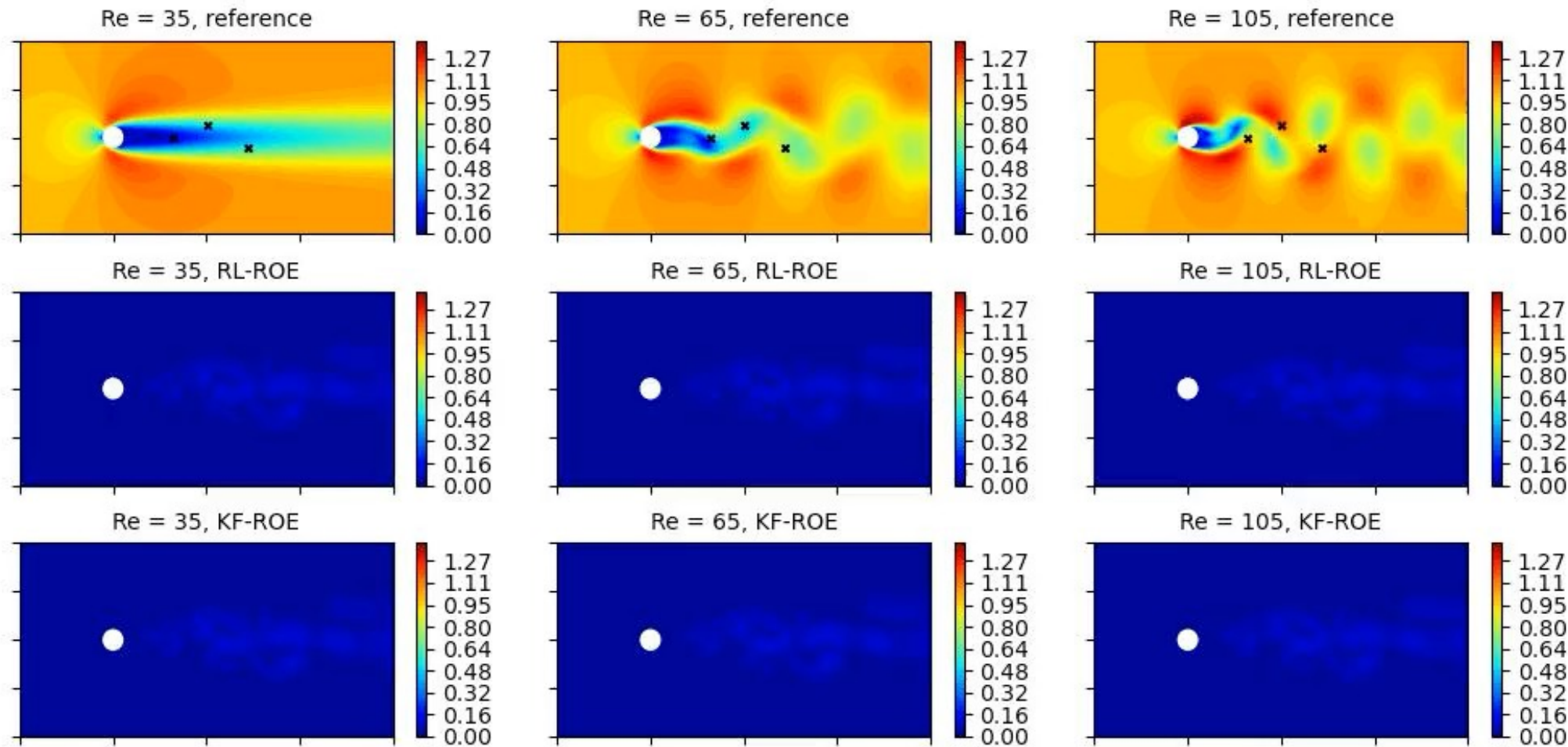
nonlinear; hybrid model-based and data-driven

$$\hat{\mathbf{x}}_k = \mathbf{A}_r \hat{\mathbf{x}}_{k-1} + \mathcal{N}(\mathbf{y}_k, \hat{\mathbf{x}}_{k-1})$$

Learn neural network  $\mathcal{N}$  offline from the training dataset using reinforcement learning

# Experimental Results: KF vs RL

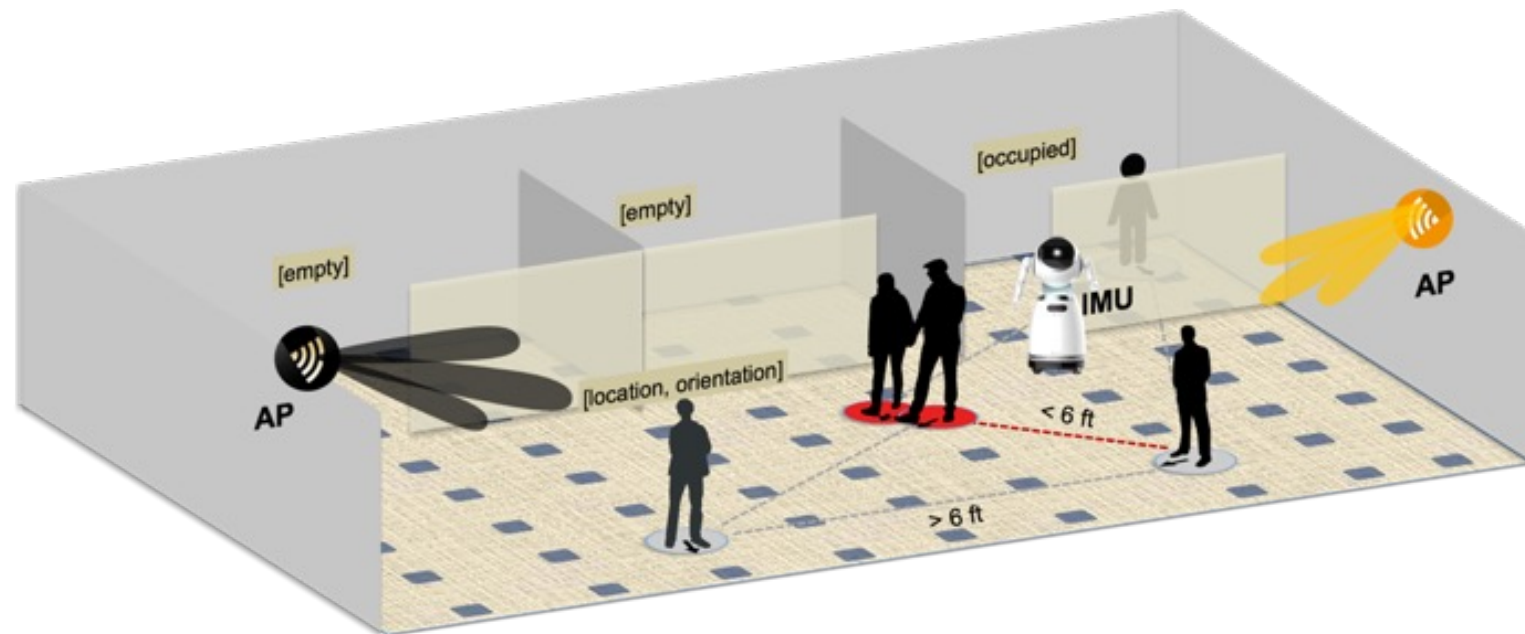
- Example with Navier-Stokes PDE: Estimate the entire flow past a cylinder with sparse velocity measurements in its wake
- The RL-ROE outperforms the KF-ROE for low number of sensors



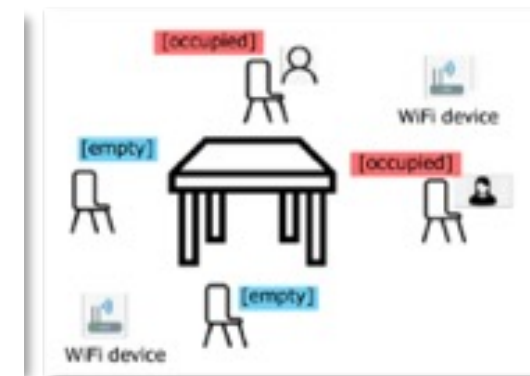
# Wi-Fi Localization and Tracking

- Reuse ambient Wi-Fi waveforms for localization and sensing applications (occupancy sensing, indoor monitoring)
- **Frame-based localization:** take one Wi-Fi frame/packet at a time and localize the object to a grid (classification) or regress its coordinate directly (regression)
- **Sequence-based localization & tracking:** take multiple consecutive frames/packets and regress the whole trajectory.
  - Existing methods use
    - either Kalman filtering-like state estimation (with a fixed dynamic model)
    - or recurrent neural networks (RNNs)

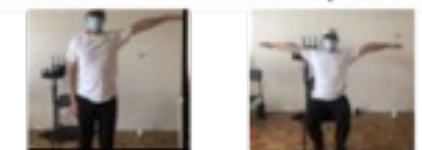
(a) Wi-Fi localization & tracking



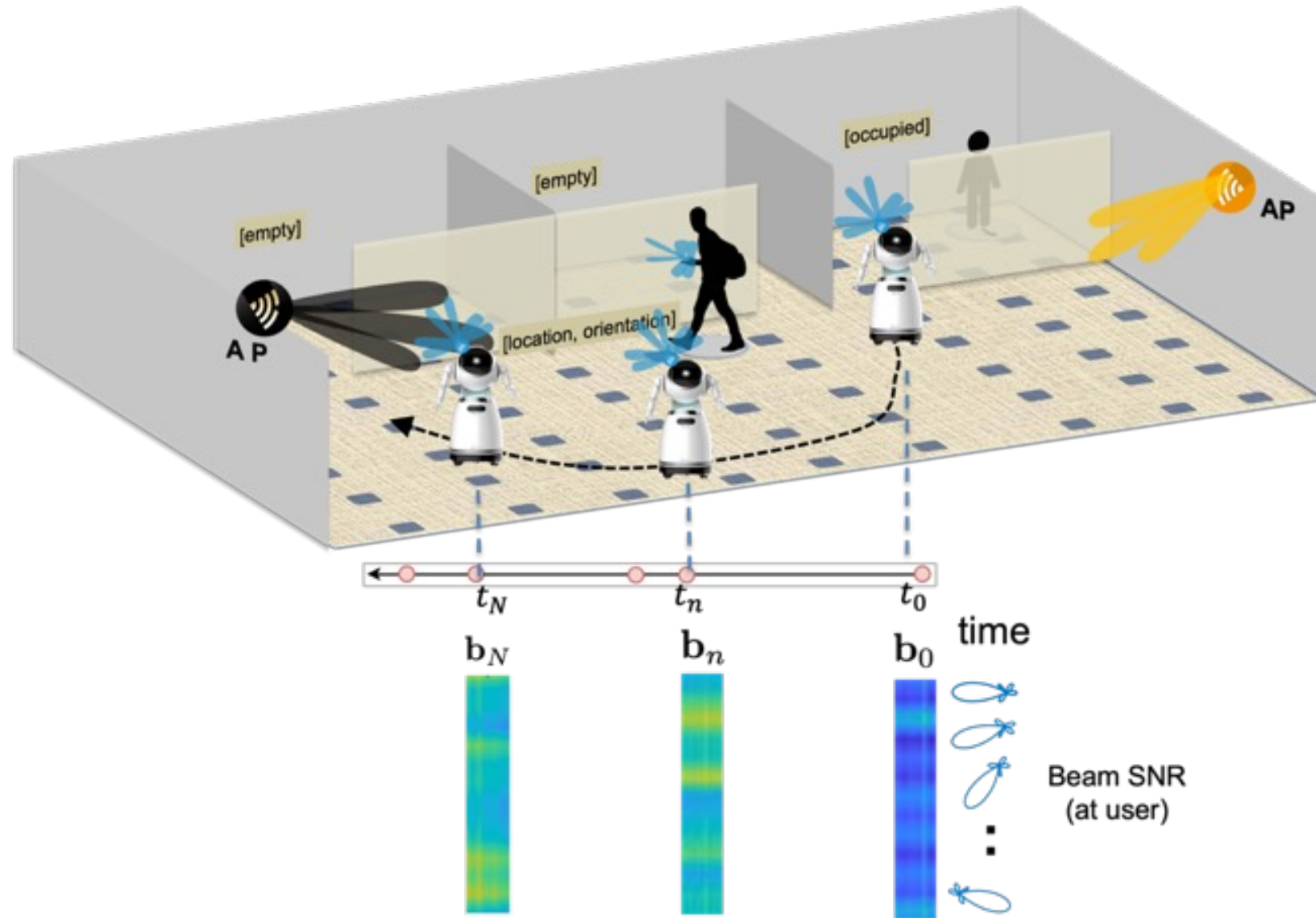
(b) Occupancy sensing



(c) Human (pose) monitoring



# mmWave Wi-Fi Trajectory Estimation

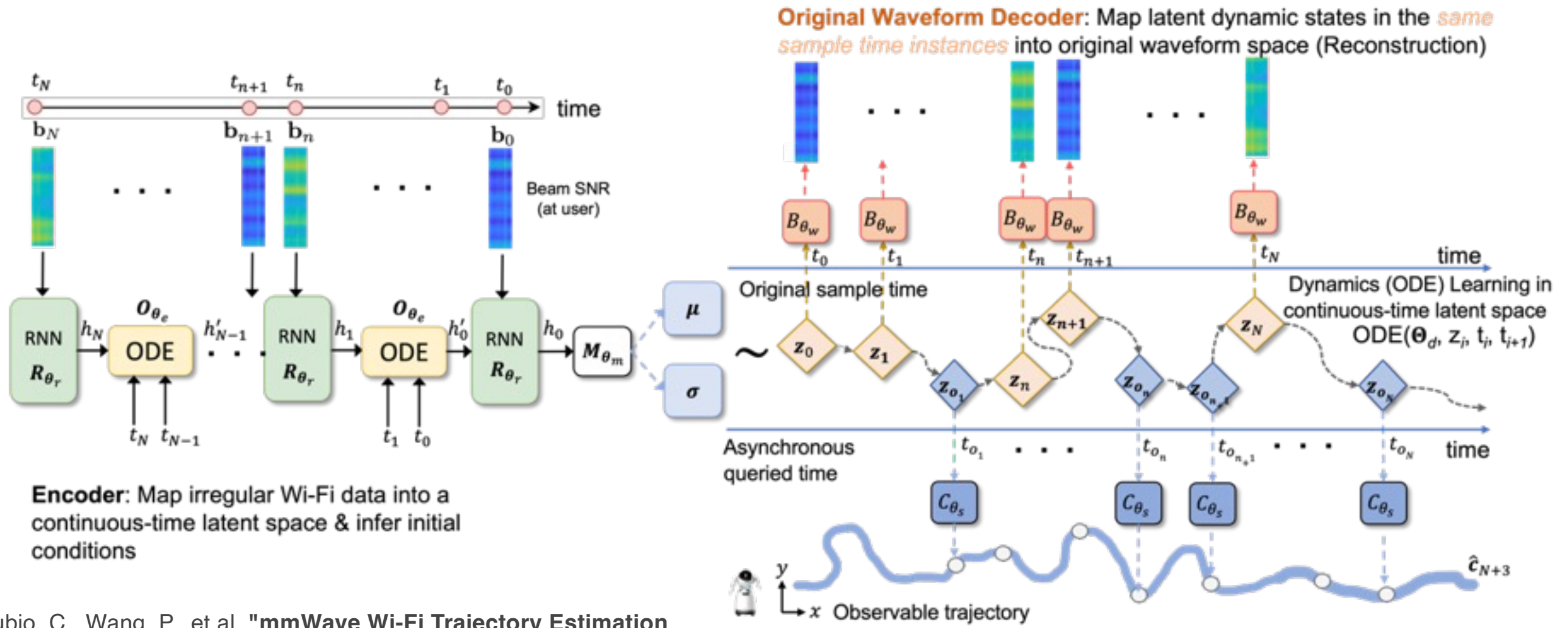


## Key Challenges

1. **Low sampling rate:** Frequent mmWave beam training results in significant overhead to Wi-Fi data transmission. Beam training rate is limited.
2. **Irregular sampling intervals:** Different users (robots, human) need to contend for channel access and lead to irregularly sampled Wi-Fi data for individual users.

# mmWave Wi-Fi Trajectory Estimation with Neural Dynamic Learning

- Learnable ordinary differential equation (ODE) to model dynamics in the high-dimensional latent space.
- ODE: address irregular sampling intervals at Encoder and allow asynchronous supervision at Decoder.
- Utilize the learned latent dynamics to improve localization performance.

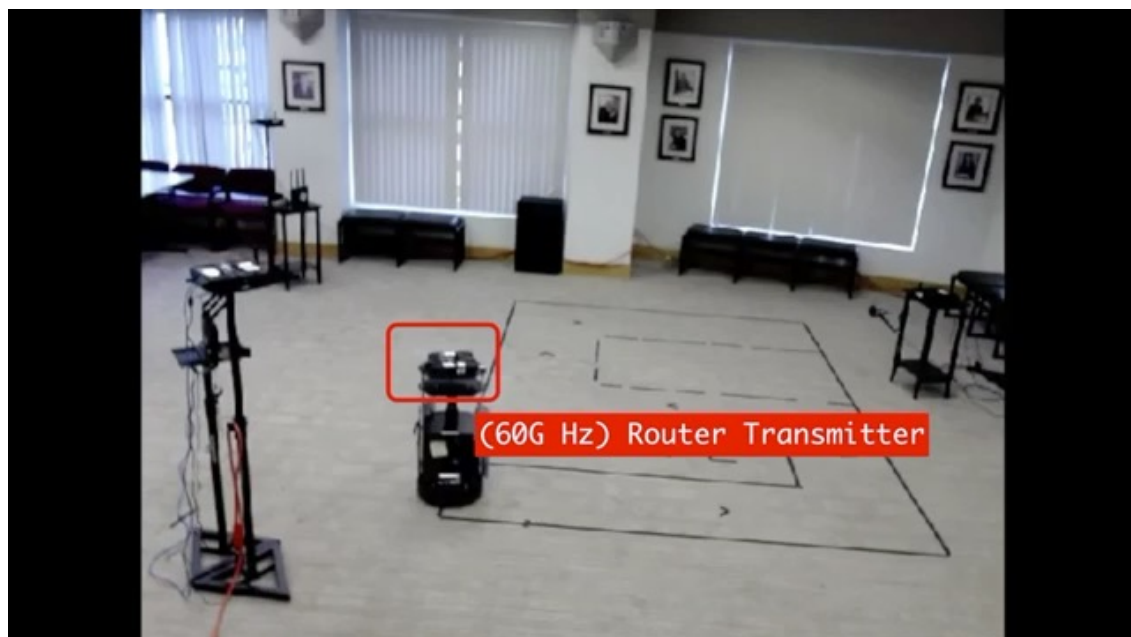


Vaca-Rubio, C., Wang, P., et al. "mmWave Wi-Fi Trajectory Estimation with Continuous-Time Neural Dynamic Learning", *ICASSP 2023*.

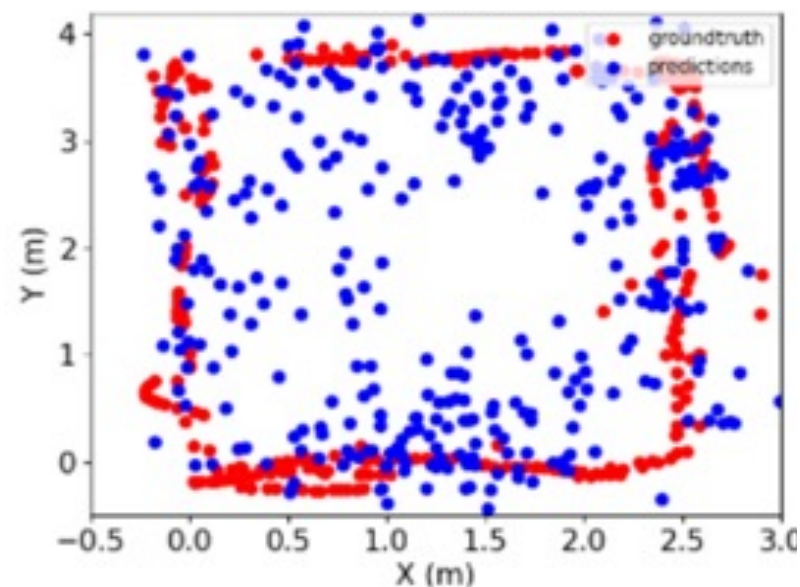
**TOP 3% PAPER AWARD**

# Performance Evaluation with In-House Experimental Data

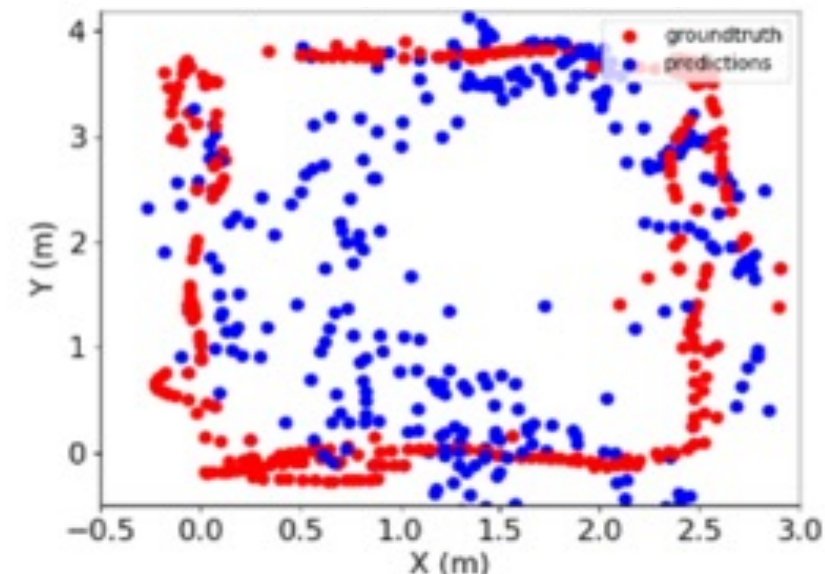
A turtle bot moving in a rectangular trajectory with on-board mmWave Wi-Fi



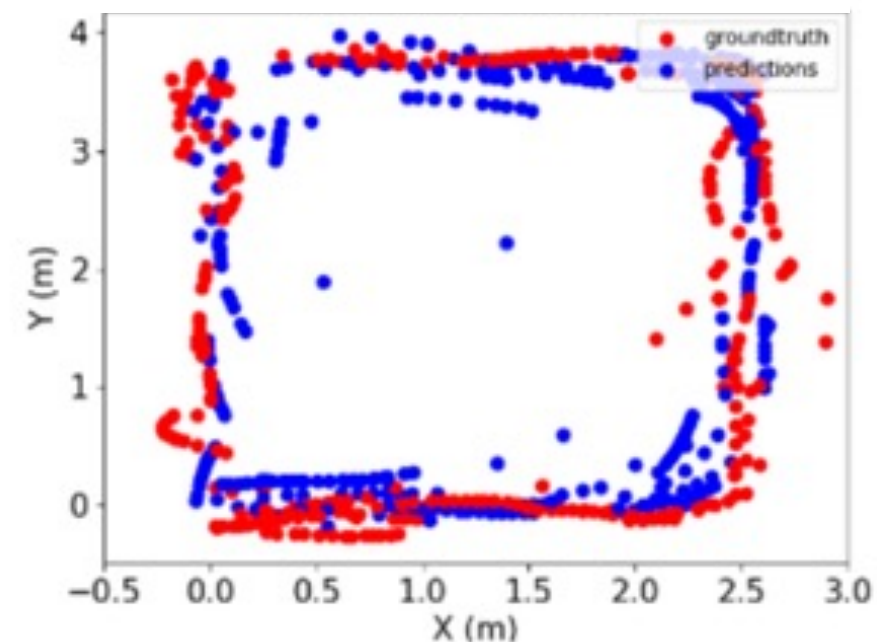
(a) Frame-based (support vector regression-SVR)



(b) Sequence-based (RNN)



(c) Sequence-based (**ours**)



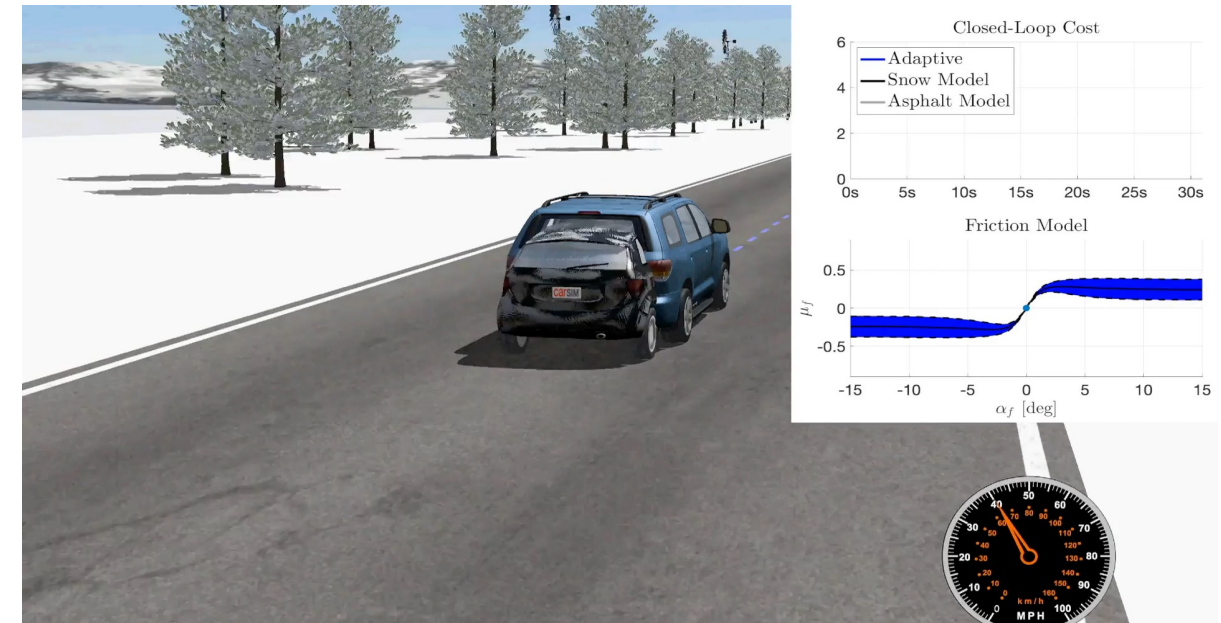
**Table 1.** Localization errors (m) on beamSNR localization dataset.

	Mean	Median	CDF@0.9
SVR	0.42	0.15	1.05
FCNNR	0.46	0.11	1.43
RNN Expdecay	0.40	0.18	1.12
RNN $\Delta t$	0.33	0.13	1.09
SDND (ours)	0.34	0.11	0.88
DDND+KL (ours)	0.26	0.11	0.74
DDND (ours)	<b>0.17</b>	<b>0.09</b>	<b>0.52</b>

## Learning friction models online


- Automated driving on varying road surfaces
- Uses efficient formulation and fast optimization solvers
- **Physics-informed** (particle filter) + **learning** (Gaussian process)

## Adaptive Stochastic MPC in CarSim Simulator

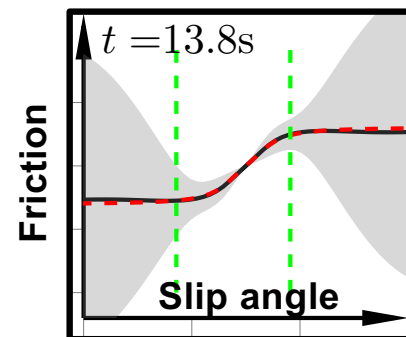


## Real-time feasible in prototyping hardware

### SMPC + Friction estimator

	$N_{MPC} = 15$		$N_{MPC} = 20$	
	$T = 0.75s$		$T = 1s$	
	$N_{PF} = 200$		$N_{PF} = 100$	
	Mean	Max	Mean	Max
QP iterations	3.65	25	6.57	25
SNMPC	16.4ms	29ms	23.1ms	37.8ms
Tire-friction estimator	10.4ms	10.5ms	5.5ms	5.6ms
Total turnaround time	26.7ms	39.4ms	28.6ms	43.3ms

### Friction estimator



Confidence

Estimates

### Model Predictive Control

$$\min_{\mathbf{x}, \mathbf{u}, \mathbf{P}} \sum_{k=0}^{N-1} l(\mathbf{x}_k, \mathbf{u}_k)$$

$$\text{s.t.} \begin{cases} \forall k \in \{0, \dots, N-1\}, \\ 0 = \mathbf{x}_{k+1} - \mathbf{f}(\mathbf{x}_k, \tilde{\mathbf{u}}_k, 0), \\ \mathbf{P}_{k+1} = \mathbf{A}_k \mathbf{P}_k \mathbf{A}_k^\top + \mathbf{B}_k \Sigma \mathbf{B}_k^\top, \quad \mathbf{P}_0 = \mathbf{P}_t, \\ 0 = \mathbf{x}_0 - \mathbf{x}_t, \\ Pr(\mathbf{h}(\mathbf{x}_k, \mathbf{u}_k) \leq 0) \geq 1 - \epsilon \end{cases}$$

### Vehicle



production sensing data

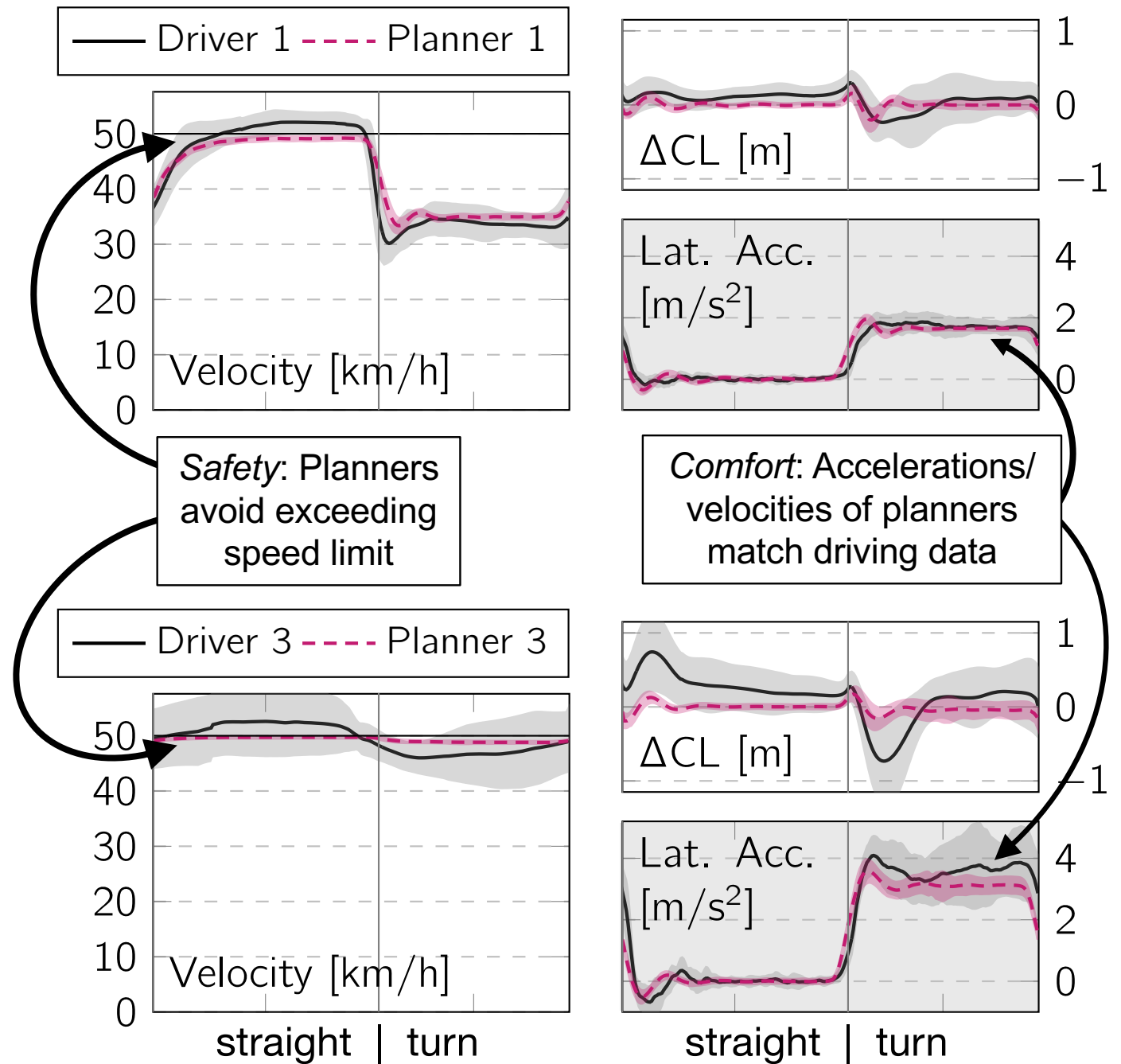
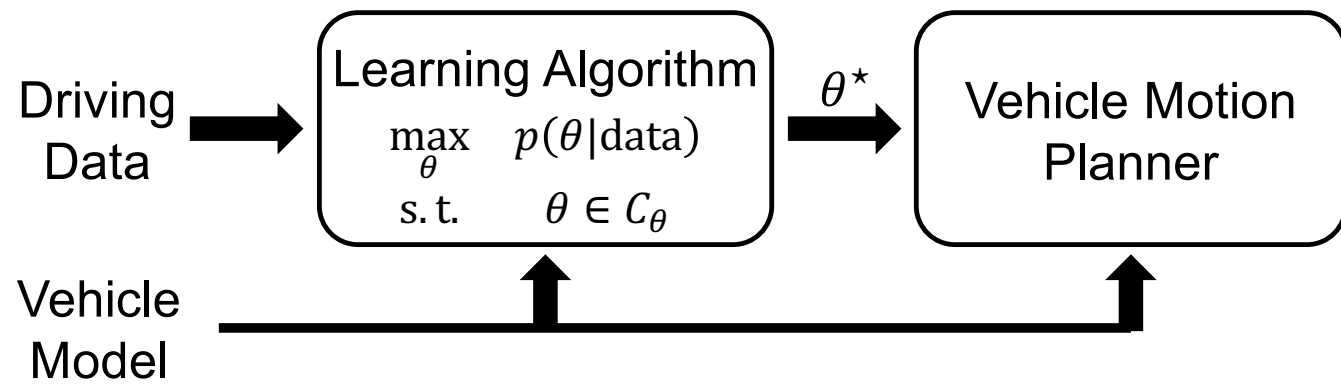
"Friction-Adaptive Stochastic Predictive Control for Autonomous Vehicle Control", Vaskov, S., Quirynen, R., Menner, M., Berntorp, K., Vehicle System Dynamics 2023

"Online Bayesian Inference and Learning of Gaussian-Process State-Space Models", K. Berntorp, Automatica 2021



# PIML for Safe and Comfortable Autonomous Driving

- **Objective: Safely adapt** vehicle behavior to **optimize passenger comfort** using driving data within **physics-informed** vehicle model and safety constraints
- Maintain Safety Guarantees
  - Fixed in controller: vehicle model, driving limits, computational structure
- Learn Performance Parameters
  - Data-driven calibration: driving objectives, comfort parameters



“Inverse learning for data-driven calibration of model-based statistical path planning”, M. Menner, K. Berntorp, M.N. Zeilinger, S. Di Cairano, *IEEE Transactions on Intelligent Vehicles*, 2021.

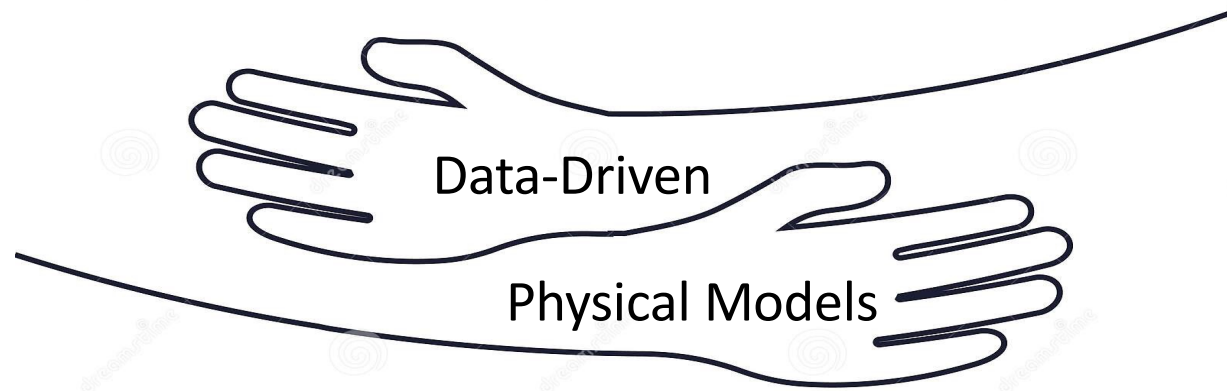
# Perspectives & Concluding Remarks

- Combining physical models and machine learning frameworks has many benefits
  - Better performance and reliability
  - More data-efficient networks
  - Allows theoretical analysis and guarantees (e.g., safety, performance, etc.)
- Reviewed several industrial applications relevant to SPS community
  - Imaging and sensing of dynamic systems
  - Trajectory estimation and tracking
  - Systems identification and motion planning
- Much more to do in this emerging field
  - Improved techniques (e.g., learning and utilizing dynamics)
  - Other physical models (e.g., geometric, optical, mechanical)
  - Different tasks (e.g., control, optimization)
  - Broader range of applications (buildings, EVs, digital twins, etc.)

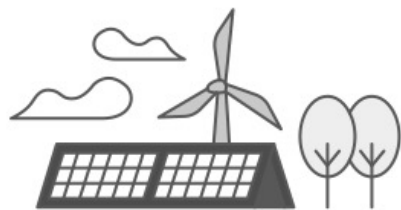


# Perspectives & Concluding Remarks

- Data-driven & physical modeling go hand in hand for many real-world engineering systems



- Encourage SPS community to further embrace this intersection
  - Very inter-disciplinary, should seek partners to push the boundaries further
    - Researcher-level to Society-level
  - Should not feel limited in scope, SP techniques have much to offer
    - Including applications that are not traditionally considered to be within SPS scope



**Carbon neutral**  
Decarbonize society



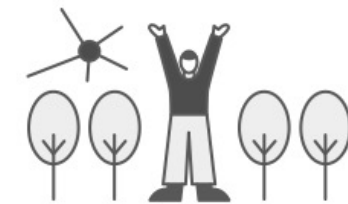
**Circular economy**  
Build a circular society



**Safety/Security**  
Resilient society



**Inclusion**  
Society that values diversity



**Well-being**  
Vibrant lives

# Thanks & Acknowledgement

## Computational Sensing



**Petros Boufounos**



**Hassan Mansour**



**Perry (Pu) Wang**



**Yanting Ma**

## Dynamics, Estimation & Control



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Benosman**



**Saviz Mowlavi**



**Ankush Chakrabarty**



**Karl Berntorp**



**Marcel Menner**



**Rien Quirynen**



**Stefano Di Cairano**